Electronic Supplementary Information

Water Oxidation by Brønsted Acid-Catalyzed *in situ* Generated Thiol Cation: Dual Function of the Acid Catalyst Leading to Transition Metal-Free Substitution and Addition Reactions of S-S Bonds

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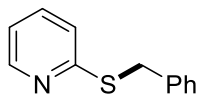
1. Experimental

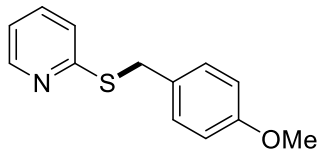
General. Unless otherwise noted, all chemicals were purchased and used without further purification. Unless otherwise specified, all reactions were carried out in sealed Schlenk tubes under air and then monitored by TLC and/or GC-MS. All products were purified by column chromatography on silica gel using petroleum ether and ethyl acetate as the eluent. Unless otherwise noted, ^{1}H and ^{13}C NMR spectra were measured on a JNM-ECZ600R/S3 (Jeol, Japan) (600 and 150 MHz for ^{1}H and ^{13}C NMR, respectively) using $CDCl_3$ as the solvent. Chemical shifts for ^{1}H and ^{13}C NMR were referred to internal Me_4Si (0 ppm) as the standard. Mass spectra were measured on an Agilent GC-MS-7890A/5975C Plus spectrometer (EI). HRMS were recorded on a LC-TOF spectrometer (Xevo G2-XS QTof) using ESI or EI techniques. Infrared spectra were measured on an Infrared spectroscopy combined with infrared microscopy (Thermo Fisher Nicolelis5). Geometry optimizations and single-point energies calculations in the ground state were using density functional theory (DFT) method with the B3LYP exchange-correlation functional in combination with the all-electron 6-31G* basis set. The nature of all stationary points was confirmed by harmonic vibrational frequency analysis. Grimme-type dispersion corrections (D3) were included throughout. Gibbs free energies of all optimized structures were calculated at 298.15 K and 1 atm. All DFT calculations were carried out using the GAUSSIAN09 package.

2. Typical Procedure and Characterization of the Products

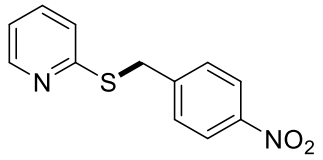
Typical procedure for the Brönsted acid-catalyzed reaction of disulfides and alcohols. The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol), benzyl alcohol **2a** (54.0 mg, 0.50 mmol, 1.0 equiv.), and $KHSO_4$ (17.0 mg, 0.125 mmol, 25 mol%) was directly sealed in a Schlenk tube (10 mL) under air and stirred at 130 ^{o}C for 12 h. The reaction mixture was then analyzed by TLC/GC-MS and purified by flash column chromatography on silica gel using ethyl acetate and petroleum ether (0~ 1/20) as the eluent, giving **3aa** in 86% isolated yield.



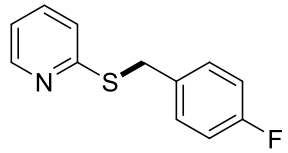
2-(Benzylthio)pyridine (3aa). Colorless oil**.** ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 4.8 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.40 (d, J = 7.2 Hz, 2H), 7.29 (dd, J = 9.6, 4.8 Hz, 2H), 7.23 (dd, J = 9.6, 4.8 Hz, 1H), 7.15 (d, J = 8.4 Hz, 1H), 7.00 – 6.95 (m, 1H), 4.43 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.9, 149.5, 138.0, 136.1, 129.1, 128.6, 127.2, 122.2, 119.7, 34.5. This compound was known: Jia, X.; Yu, L.; Liu, J.; Xu, Q.; Sickert, M.; Chen, L.; Lautens, M. *Green Chem.* **2014**, *16*, 3444.



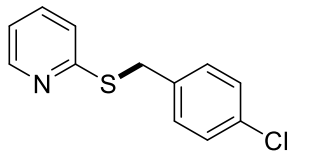
2-((4-Methoxybenzyl)thio)pyridine (3ab). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 4.8 Hz, 1H), 7.47 – 7.44 (m, 1H), 7.33 – 7.31 (m, 2H), 7.14 (dd, J = 4.2, 4.2 Hz, 1H), 7.00 – 6.95 (m, 1H), 6.83 – 6.80 (m, 2H), 4.38 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 158.8, 149.5, 136.1, 130.2, 129.9, 122.2, 119.6, 114.0, 55.4, 34.1. This compound was known: Han, X.; Wu, J. *Org. Lett.* **2010**, *12*, 5780.



2-((4-Nitrobenzyl)thio)pyridine (3ac). Brown solid, m.p. 84 – 85 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (dd, J = 6.0, 1.8 Hz, 1H), 8.14 – 8.09 (m, 2H), 7.56 (dd, J = 9.0, 1.8 Hz, 2H), 7.49 – 7.44 (m, 1H), 7.16 – 7.12 (m, 1H), 7.02 – 6.97 (m, 1H), 4.49 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.2, 149.5, 147.0, 146.7, 136.3, 129.9, 123.7, 122.5, 120.2, 33.4. This compound was known: Goriya, Y.; Ramana, C. V. *Tetrahedron* **2010**, *66*, 7642.

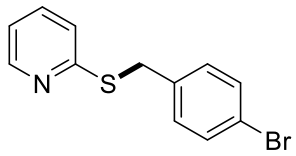


2-((4-Fluorobenzyl)thio)pyridine (3ad). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 – 8.43 (m, 1H), 7.47 – 7.43 (m, 1H), 7.39 – 7.34 (m, 2H), 7.14 (d, J = 8.4 Hz, 1H), 7.00 – 6.94 (m, 3H), 4.40 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.0 (d, J = 245.2 Hz), 158.5, 149.5, 136.1, 134.0 (d, J = 2.5 Hz), 130.6 (d, J = 8.2 Hz), 122.3, 119.8, 115.4 (d, J = 21.4 Hz), 33.6. This compound was known: Dean, W. M.; Šiaučiulis, M.; Storr, T. E.; Lewis, W.; Stockman, R. A. *Angew. Chem. Int. Ed.* **2016**, *55*, 10013.

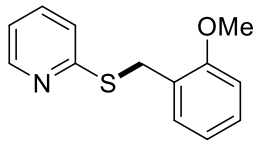


2-((4-Chlorobenzyl)thio)pyridine (3ae). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 4.8 Hz, 1H), 7.44 (dd, J = 7.8, 7.8 Hz, 1H), 7.33 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 7.13 (d, J = 7.8 Hz, 1H), 6.98 (d, J = 6.0 Hz, 1H), 4.39 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ

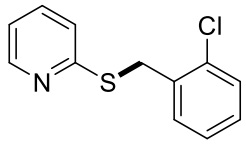
158.3, 149.5, 136.9, 136.1, 132.9, 130.4, 128.7, 122.3, 119.9, 33.6. HRMS (ESI) for $C_{12}H_{11}ClNS$ (M+H) Calcd: 236.0301; found: 236.0285. This compound was known: Tresoldi, G.; Lo Schiavo, S.; Lanza, S.; Cardiano, P. *Eur. J. Inorg. Chem.* 2002, 181.



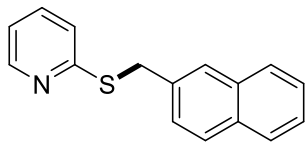
2-((4-Bromobenzyl)thio)pyridine (3af). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (dd, J = 4.8, 1.8 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.40 – 7.38 (m, 2H), 7.29 – 7.26 (m, 2H), 7.13 (dd, J = 4.2, 4.2 Hz, 1H), 7.00 – 6.96 (m, 1H), 4.37 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.2, 149.5, 137.5, 136.1, 131.6, 130.8, 122.3, 121.0, 119.8, 33.7. This compound was known: Haviv, F.; DeNet, R. W.; Michaels, R. J.; Ratajczyk, J. D.; Carter, G. W.; Young, P. R. *J. Med. Chem.* **1983**, *26*, 218.



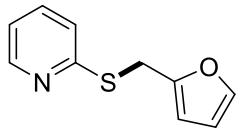
2-((2-Methoxybenzyl)thio)pyridine (3ag). Colorless oil**.** ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, J = 4.5 Hz, 1H), 7.44– 7.40 (m, 2H), 7.21 (dd, J = 7.8, 1.2 Hz, 1H), 7.14 (d, J = 8.4 Hz, 1H), 6.97 – 6.94 (m, 1H), 6.88 – 6.85 (m, 2H), 4.47 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.6, 157.6, 149.4, 135.9, 130.6, 128.6, 126.3, 122.2, 120.5, 119.4, 110.6, 55.6, 29.1. This compound was known: Pathak, A. K.; Pathak, V.; Seitz, L. E.; Suling, W. J.; Reynolds, R. C. *J. Med. Chem.* **2004**, *47*, 1273.



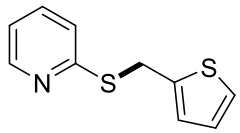
2-((2-Chlorobenzyl)thio)pyridine (3ah). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (dd, J = 4.8, 2.4 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.47 – 7.45 (m, 1H), 7.38 – 7.33 (m, 1H), 7.19 – 7.14 (m, 3H), 6.99 (dd, J = 7.8, 4.8 Hz, 1H), 4.56 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.4, 149.4, 136.1, 136.0, 134.4, 131.1, 129.6, 128.6, 126.9, 122.4, 119.7, 31.9. This compound was known: Ma, X.; Yu, L.; Su, C.; Yang, Y.; Li, H.; Xu, Q. *Adv. Synth. Catal.* **2017**, *359*, 1649.



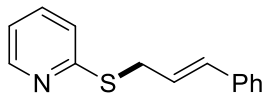
2-((Naphthalen-1-ylmethyl)thio)pyridine (3ai). White solid. 124 – 125 ^{o}C ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, J = 4.8 Hz, 1H), 7.85 (s, 1H), 7.79 (t, J = 8.4 Hz, 3H), 7.53 (dd, J = 8.4, 1.2 Hz, 1H), 7.49 – 7.39 (m, 3H), 7.17 (d, J = 8.4 Hz, 1H), 6.99 (dd, J = 7.2, 4.8 Hz, 1H), 4.60 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.8, 149.5, 136.1, 135.5, 133.4, 132.7, 128.4, 127.8, 127.7, 127.6, 127.3, 126.2, 125.9, 122.3, 119.8, 34.8. HRMS (ESI) for $C_{16}H_{14}NS$ (M+H) Calcd: 252.0847; found: 252.0864. Ma, X.; Yu, J.; Yan, R.; Yan, M.; Xu, Q. *J. Org. Chem.* **2019**, *84*, 11294.



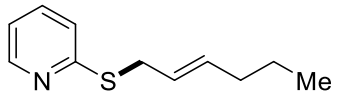
2-((Furan-2-ylmethyl)thio)pyridine (3aj). Colorless oil**.** ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (dd, J = 4.8, 1.8 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.32 (d, J = 2.4 Hz, 1H), 7.17 (dd, J = 8.4, 1.2 Hz, 1H), 7.00 – 6.97 (m, 1H), 6.27 (dd, J = 3.0, 1.8 Hz, 1H), 6.23 (d, J = 3.0 Hz, 1H), 4.47 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.0, 149.5, 142.1, 136.1, 122.5, 119.8, 110.6, 107.8, 29.8. This compound was known: Dean, W. M.; Šiaučiulis, M.; Storr, T. E.; Lewis, W.; Stockman, R. A. *Angew. Chem. Int. Ed.* **2016**, *55*, 10013.



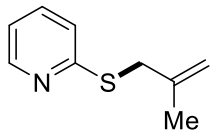
2-((Thiophen-2-ylmethyl)thio)pyridine (3ak). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (dd, J = 4.8, 0.6 Hz, 1H), 7.53 – 7.44 (m, 1H), 7.20 – 7.11 (m, 2H), 7.01 – 6.96 (m, 1H), 6.89 (dd, J = 5.4, 3.6 Hz, 1H), 4.65 (s, 2H) ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.0, 149.3, 141.1, 136.0, 126.6, 126.3, 124.8, 122.3, 119.7, 28.8. This compound was known: Ma, X.; Yu, L.; Su, C.; Yang, Y.; Li, H.; Xu, Q. *Adv. Synth. Catal.* **2017**, *359*, 1649.



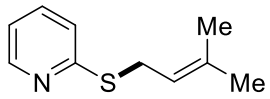
2-(Cinnamylthio)pyridine (3al). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 4.2 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.35 – 7.16 (m, 6H), 7.01 – 6.96 (m, 1H), 6.61 (d, J = 15.6 Hz, 1H), 6.33 (dt, J = 15.6, 7.2 Hz, 1H), 4.01 (dd, J = 7.2, 1.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.6, 149.6, 136.9, 136.1, 132.8, 128.6, 127.6, 126.4, 125.4, 122.5, 119.7, 32.8. This compound was known: Santos, S.; Quignard, F.; Sinou, D.; Choplin, A. *Top. Catal.* **2000**, *13*, 311.



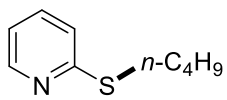
(E)-2-(Hex-2-en-1-ylthio)pyridine (3am). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 4.8 Hz, 1H), 7.49 – 7.42 (m, 1H), 7.15 (d, J = 7.2 Hz, 1H), 6.99 – 6.93 (m, 1H), 5.71 – 5.64 (m, 1H), 5.58 – 5.52 (m, 1H), 3.77 (d, J = 7.2 Hz, 2H), 1.97 (dd, J = 14.4, 7.2 Hz, 2H), 1.34 (dd, J = 14.4, 7.2 Hz, 2H), 0.84 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 149.5, 136.0, 134.4, 125.1, 122.4, 119.5, 34.5, 32.7, 22.4, 13.7. This compound was known: Goux, C.; Lhoste, P.; Sinou, D. *Tetrahedron* **1994**, *50*, 10321.



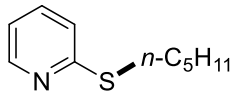
2-((2-Methylallyl)thio)pyridine (3an). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 4.8 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.17 (d, J = 7.8 Hz, 1H), 6.96 (dd, J = 7.2, 4.8 Hz, 1H), 5.01 (s, 1H), 4.85 (s, 1H), 3.84 (s, 2H), 1.84 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 149.5, 141.4, 136.0, 122.4, 119.6, 113.8, 37.3, 21.6. This compound was known: Galaka, T.; Casal, M. F.; Storey, M.; Li, C.; Chao, M. N.; Szajnman, S. H.; Docampo, R.; Moreno, S. N. J.; Rodriguez, J. B. *Molecules* **2017**, *22*, 82.



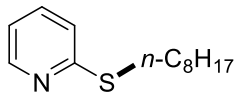
2-((3-Methylbut-2-en-1-yl)thio)pyridine (3ao). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 4.8 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.14 (d, J = 7.8 Hz, 1H), 6.95 (dd, J = 7.2, 4.8 Hz, 1H), 5.35 (t, J = 7.8 Hz, 1H), 3.80 (d, J = 7.8 Hz, 2H), 1.72 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 149.5, 141.4, 136.0, 122.4, 119.6, 113.8, 28.6, 25.8 14.2. This compound was known: Goux, C.; Lhoste, P.; Sinou, D. *Tetrahedron*, **1994**, *50*, 10321.



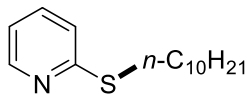
2-(Butylthio)pyridine (3ap). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 – 8.37 (m, 1H), 7.49 – 7.41 (m, 1H), 7.15 (d, J = 7.8 Hz, 1H), 6.97 – 6.91 (m, 1H), 3.15 (t, J = 7.2 Hz, 2H), 1.70 – 1.65 (m, 2H), 1.50 – 1.44 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 149.5, 135.9, 122.2, 119.3, 31.5, 29.9, 22.2, 13.8. This compound was known: Nath, D.; Skilbeck, M. C.; Coldham, I.; Fleming, F. F. *Org. Lett.* **2014**, *16*, 62.



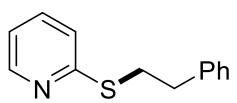
2-(Pentylthio)pyridine (3aq). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, J = 4.8 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.15 (d, J = 7.8 Hz, 1H), 6.98 – 6.90 (m, 1H), 3.14 (t, J = 7.8 Hz, 2H), 1.73 – 1.67 (m, 2H), 1.44 – 1.39 (m, 2H), 1.36 – 1.32 (m, 2H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 149.5, 135.9, 122.2, 119.2, 31.2, 30.2, 29.1, 22.4, 14.1. This compound was known: Xiao, Z.; Wang, L.; Wei, J.; Ran, C.; Liang, S.H.; Shang, J.; Chen, G.-Y.; Zheng, C. *Chem. Commun.* **2020**, *56*, 4164.



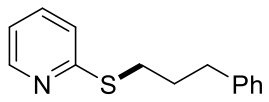
2-(Octylthio)pyridine (3ar). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (dd, J = 4.8, 2.4 Hz, 1H), 7.45 (dt, J = 7.8, 1.8 Hz, 1H), 7.18 – 7.12 (m, 1H), 6.98 – 6.92 (m, 1H), 3.16 – 3.12 (m, J 2H), 1.69 (dt, J = 15.0, 7.2 Hz, 2H), 1.45 – 1.41 (m, 2H), 1.36 – 1.17 (m, 8H), 0.88 (t, J = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 149.5, 135.9, 122.2, 119.3, 31.9, 30.2, 29.4, 29.3, 29.1, 22.8, 14.2. This compound was known: Duan, Z.; Ranjit, S.; Zhang, P.; Liu, X. *Chem.–Eur. J.* **2009**, *15*, 3666.



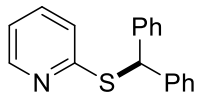
2-(Decyl)pyridine (3as). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (dd, J = 4.8, 1.8 Hz, 1H), 7.48 – 7.42 (m, 1H), 7.15 (d, J = 7.8 Hz, 1H), 6.98 – 6.91 (m, 1H), 3.16 – 3.12 (m, 2H), 1.73 – 1.63 (m, 2H), 1.45 – 1.40 (m, 2H), 1.35 – 1.20 (m, 12H), 0.86 (t, J = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 149.5, 135.9, 122.2, 119.2, 32.0, 30.2, 29.7, 29.42, 29.39, 29.3, 29.1, 22.8, 14.2. This compound was known: Brussaard, Y.; Olbrich, F.; Schaumann, E. *Inorg. Chem.* **2013**, *52*, 13160.



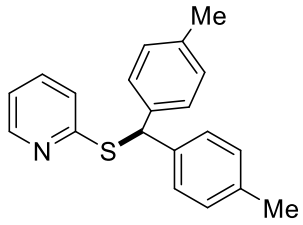
2-(Phenethylthio)pyridine (3at). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 – 8.42 (m, 1H), 7.49 – 7.43 (m, 1H), 7.37 – 7.26 (m, 4H), 7.22 (dd, J = 7.2, 7.2 Hz, 1H), 7.17 (d, J = 7.2 Hz, 1H) 6.97 (dd, J = 7.8, 4.8 Hz, 1H), 3.43 (t, J = 7.8 Hz, 2H), 3.00 (t, J = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.0, 149.6, 140.7, 135.9, 128.8, 128.5, 126.5, 122.5, 119.4, 35.9, 31.5. This compound was known: Qiao, Z.; Wei, J.; Jiang, X. *Org. Lett.* **2014**, *16*, 1212.



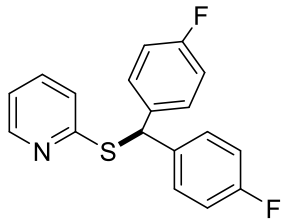
2-((3-Phenylpropyl)thio)pyridine (3au). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 4.2 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.32 – 7.25 (m, 2H), 7.22 – 7.14 (m, 4H), 7.03 – 6.89 (m, 1H), 3.28 – 3.11 (m, 2H), 2.88 – 2.74 (m, 2H), 2.09 – 2.00 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 149.6, 141.6, 136.0, 128.6, 128.5, 126.0, 122.3, 119.4, 35.0, 31.1, 29.6. This compound was known: Legarda, P. D.; García-Rubia, A.; Arrayás, R. G.; Carretero, J. C. *Adv. Synth. Catal.* **2016**, *358*, 1065.



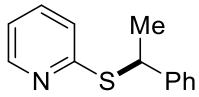
2-(Benzhydrylthio)pyridine (3av). White solid. 69 – 70 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, J = 2.4 Hz, 1H), 7.48 (d, J = 7.2 Hz, 4H), 7.42 – 7.39 (m, 1H), 7.34 – 7.25 (m, 4H), 7.22 (dd, J = 7.2, 7.2 Hz, 2H), 7.11 (d, J = 7.8 Hz, 1H), 6.93 (dd, J = 6.6, 5.4 Hz, 1H), 6.35 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.4, 149.5, 141.4, 136.3, 128.7, 128.6, 127.2, 122.4, 52.8. This compound was known: Duffy, B. C.; Howard, K. T.; Chisholm, J. D. *Tetrahedron Lett.* **2015**, *56*, 3301.



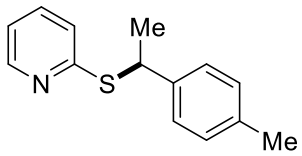
2-((Di-p-tolylmethyl)thio)pyridine (3aw). White solid. 86 – 87 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 – 8.35 (m, 1H), 7.42 – 7.37 (m, 1H), 7.35 (d, J = 7.8 Hz, 4H), 7.09 (d, J = 7.8 Hz, 5H), 6.92 (dd, J = 7.8, 4.8 Hz, 1H), 6.24 (s, 1H), 2.30 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.9, 149.5, 138.6, 136.8, 136.2, 129.3, 128.5, 122.3, 119.8, 52.3, 21.2. IR (KBr): v 2954, 2921, 2853, 1574, 1556, 1508, 1453, 1413, 1157, 1146, 1120, 1043, 808, 782, 761, 750 cm^{-1}. HRMS (ESI) for $C_{20}H_{20}NS$ (M+H) Calcd: 306.1316; found: 306.1327.



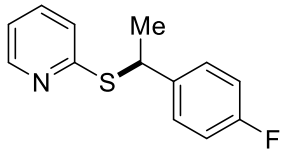
2-((Bis(4-fluorophenyl)methyl)thio)pyridine (3ax). White solid. 60 – 61 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 – 8.35 (m, 1H), 7.41 – 7.45 (m, 1H), 7.41 – 7.36 (m, 4H), 7.10 (d, J = 8.4 Hz, 1H), 6.99 – 6.94 (m, 5H), 6.32 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.9 (d, J = 246.5 Hz), 157.8, 149.6, 137.1, 136.3, 130.2 (d, J = 8.2 Hz), 122.5, 120.1, 115.5 (d, J = 21.6 Hz). IR (KBr): v 2994, 2924, 2853, 1600, 1575, 1554, 1503, 1465, 1453, 1412, 1221, 1157, 1148, 1121, 1099, 864, 826, 821, 793, 779, 751, 732 cm^{-1}. HRMS (ESI) for $C_{18}H_{14}F_2NS$ (M+H) Calcd: 314.0185; found: 314.0174.



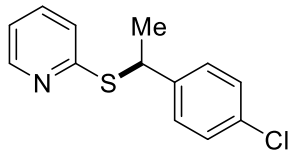
2-((1-Phenylethyl)thio)pyridine (3ay). Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 4.8 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.30 (dd, J = 7.2, 7.2 Hz, 2H), 7.22 (dd, J = 7.2, 7.2 Hz, 1H), 7.10 (d, J = 7.8 Hz, 1H), 6.96 (dd, J = 6.6, 5.4 Hz 1H), 5.10 (q, J = 7.2 Hz, 1H), 1.74 (d, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.9, 149.6, 143.4, 136.1, 128.6, 127.5, 127.2, 122.9, 119.7, 43.7, 22.7. This compound was known: Ma, H.; Ren, X.; Zhou, X.; Ma, C.; He, Y.; Huang, G. *Tetrahedron Lett.* **2015**, *56*, 6022.



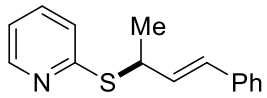
2-((1-(p-Tolyl)ethyl)thio)pyridine (3az). Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 4.8 Hz, 1H), 7.46 – 7.38 (m, 1H), 7.33 (d, J = 7.8 Hz, 2H), 7.12 – 7.07 (m, 3H), 7.00 – 6.89 (m, 1H), 5.05 (q, J = 7.2 Hz, 1H), 2.30 (s, 3H), 1.72 (d, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 149.6, 140.3, 136.9, 136.0, 129.3, 127.3, 122.9, 119.7, 43.4, 22.7, 21.2. This compound was known: Ma, H.; Ren, X.; Zhou, X.; Ma, C.; He, Y.; Huang, G. *Tetrahedron Lett.* **2015**, *56*, 6022.



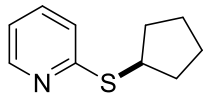
2-((1-(4-Fluorophenyl)ethyl)thio)pyridine (3aB). Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 (d, J = 4.8 Hz, 1H), 7.46 – 7.35 (m, 3H), 7.08 (d, J = 8.4 Hz, 1H), 6.99 – 6.91 (m, 3H), 5.09 (q, J = 7.2 Hz, 1H), 1.71 (d, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.9 (d, J = 245.2 Hz), 158.6, 149.6, 139.2, 136.1, 129.0 (d, J = 8.2 Hz), 123.0, 119.9, 115.3 (d, J = 21.5 Hz), 42.9, 22.7. This compound was known: Ma, H.; Ren, X.; Zhou, X.; Ma, C.; He, Y.; Huang, G. *Tetrahedron Lett.* **2015**, *56*, 6022.



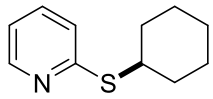
2-((1-(4-Chlorophenyl)ethyl)thio)pyridine (3aC). Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, J = 4.8 Hz, 1H), 7.45 – 7.42 (m, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.26 – 7.23 (m, 2H), 7.08 (d, J = 8.4 Hz, 1H), 6.96 (dd, J = 7.2, 4.8 Hz, 1H), 5.08 (q, J = 7.2 Hz, 1H), 1.69 (d, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.4, 149.6, 142.2, 136.2, 132.8, 128.9, 128.6, 123.0, 119.9, 42.9, 22.5. This compound was known: Ma, H.; Ren, X.; Zhou, X.; Ma, C.; He, Y.; Huang, G. *Tetrahedron Lett.* **2015**, *56*, 6022.



(*E*)-2-((4-Phenylbut-3-en-2-yl)thio)pyridine (3aD). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 4.2 Hz, 1H), 7.48 – 6.44 (m, 1H), 7.32 (d, J = 7.8 Hz, 2H), 7.30 – 7.25 (m, 2H), 7.21 – 7.16 (m, 2H), 7.00 – 6.94 (m, 1H), 6.55 (d, J = 15.6 Hz, 1H), 6.31 (dd, J = 15.6, 7.8 Hz, 1H), 4.72 – 6.67 (m, 1H), 1.59 (d, J = 6.8 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.6, 149.6, 137.0, 136.1, 131.3, 130.0, 128.6, 127.5, 126.4, 123.5, 119.9, 41.9, 20.5. This compound was known: Siddaraju, Y.; Prabhu, K. R. *J. Org. Chem.* **2018**, *83*, 11145.

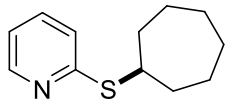


2-(Cyclopentylthio)pyridine (3aE). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 4.8 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.15 (d, J = 8.4 Hz, 1H), 7.01 – 6.86 (m, 1H), 4.07 – 3.96 (m, 1H), 2.24 – 2.13 (m, 2H), 1.81 – 1.74 (m, 2H), 1.67 – 1.60 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.6, 149.6, 135.9, 122.3, 119.2, 43.1, 33.6, 25.0. This compound was known: Wang, Q.; Zhu, B.; Yang, G.; Ma, X.; Xu, Q. *Chin. J. Org. Chem.* **2021**, *41*, 1193.

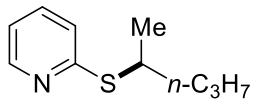


2-(Cyclohexylthio)pyridine (3aF). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 3.6 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.14 (dd, J = 5.4, 5.4 Hz,1H), 6.98 – 6.89 (m, 1H), 3.79 (d, J = 3.6 Hz, 1H), 2.11 – 2.04 (m, 2H), 1.80 – 1.71 (m, 2H), 1.64 – 1.58 (m, 1H), 1.48 – 1.42 (m, 4H), 1.32 – 1.25 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 149.6, 136.0, 123.0, 119.4, 43.0, 33.4, 26.1, 25.9. This compound was known: Zhao, J.; Fang, H.; Han, J.; Pan, Y.; Li, G. *Adv. Synth.*

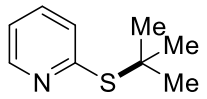
Catal. **2014**, *356*, 2719.



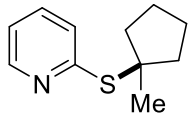
2-(Cycloheptylthio)pyridine (3aG). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (dd, J = 4.8, 1.9 Hz), 7.48 – 7.41 (m, 1H), 7.16 – 7.10 (m, 1H), 6.97 – 6.89 (m, 1H), 3.97 (tt, J = 9.0, 4.2 Hz, 1H), 2.12 – 2.07 (m, 2H), 1.74 – 1.66 (m, 4H), 1.64 – 1.55 (m, 6H).. ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.8 149.6, 135.9, 122.9, 119.3, 44.7, 34.9, 28.5, 26.0. This compound was known: Wang, Q.; Zhu, B.; Yang, G.; Ma, X.; Xu, Q. *Chin. J. Org. Chem.* **2021**, *41*, 1193.



2-(Pentan-2-ylthio)pyridine (3aH). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 4.2 Hz, 1H), 7.46 – 6.42 (m, 1H), 7.14 (d, J = 8.4 Hz, 1H), 7.02 – 6.88 (m, 1H), 3.90 (dq, J = 13.8, 6.6 Hz, 1H), 1.69 – 1.65 (m, 1H), 1.60 – 1.55 (m, 1H), 1.49 – 1.42 (m, 2H), 1.38 (d, J = 6.6 Hz, 3H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 149.6, 135.9, 123.0, 119.3, 39.7, 38.9, 21.5, 20.4, 14.1. This compound was known: Xiao, Z.; Wang, L.; Wei, J.; Ran, C.; Liang, S.H.; Shang, J.; Chen, G.-Y.; Zheng, C. *Chem. Commun.* **2020**, *56*, 4164.

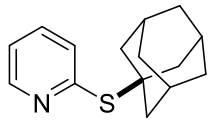


2-(Tert-butylthio)pyridine (3aI). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, J = 4.8 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.32 (d, J = 7.8 Hz, 1H), 7.10 – 7.03 (m, 1H), 1.49 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.5, 149.6, 136.1, 127.7, 121.0, 47.7, 31.2. This compound was known: Xiao, Z.; Wang, L.; Wei, J.; Ran, C.; Liang, S.H.; Shang, J.; Chen, G.-Y.; Zheng, C. *Chem. Commun.* **2020**, *56*, 4164.

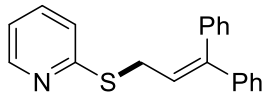


2-((1-Methylcyclopentyl)thio)pyridine (3aJ). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (dd, J = 4.8, 1.2 Hz, 1H), 7.49 – 7.45 (m, 1H), 7.33 – 7.21 (m, 1H), 7.05 – 6.97 (m, 1H), 2.15 – 2.05 (m, 2H), 1.85 – 1.79 (m, 2H), 1.76 – 1.67 (m, 4H), 1.62 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.6, 135.9, 126.0, 120.3, 41.0 29.8, 28.8, 24.4. IR (KBr): v2955, 2923, 2853, 1578, 1556, 1452, 1413, 1123, 757, 733 cm^{-1}. HRMS (ESI) for $C_{11}H_{16}NS$ (M+H) Calcd: 194.1003;

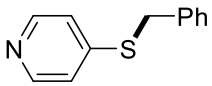
found: 193.9992.



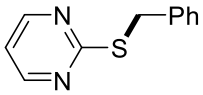
2-(1-Adamantanylthio)pyridine (3aK). White solid. 78 – 79 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (d, *J* = 4.8 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.37 (d, *J* = 7.2 Hz, 1H), 7.12 – 7.06 (m, 1H), 2.05 (d, *J* = 2.4 Hz, 6H), 2.02 (s, 3H), 1.66 (t, *J* = 2.4 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.8, 149.7, 136.1, 129.2, 121.5, 50.1, 43.7, 36.3, 30.1. This compound was known: Ho, J.; Zheng, J.; Meana-Pañeda, R.; Truhlar, D. G.; Ko, E. J.; Savage, G. P.; Tsanaktsidis, J. *J. Org. Chem.* **2013**, *78*, 6677.



2-((3,3-Diphenylallyl)thio)pyridine (3aL). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 4.8 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.40 (dd, *J* = 7.2, 7.2 Hz, 2H), 7.34 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.27 – 7.20 (m, 7H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.96 (dd, *J* = 6.6, 4.8 Hz, 1H), 6.28 (t, *J* = 7.8 Hz, 1H), 3.91 (d, *J* = 7.8 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.9, 149.5, 144.4, 142.1, 139.2, 136.0, 130.1, 128.4, 128.2, 127.63, 127.55, 127.51, 124.3, 122.2, 119.5, 30.1. IR (KBr): *v* 3054, 2972, 2927, 1598, 1577, 1444, 1413, 1123, 1043, 757, 696 cm^{-1}. HRMS (ESI) for $C_{20}H_{18}NS$ (M+H) Calcd: 304.1160; found: 304.1172.

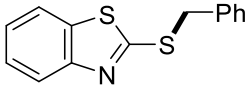


4-(Benzylthio)pyridine (3ba). White solid. 60 – 61 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 – 8.32 (m, 2H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.14 – 7.09 (m, 2H), 4.20 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.4, 149.1, 135.6, 128.9, 128.8, 127.8, 120.9, 35.8. This compound was known: Ma, X.; Yu, L.; Su, C.; Yang, Y.; Li, H.; Xu, Q. *Adv. Synth. Catal.* **2017**, *359*, 1649.

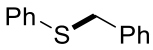


2-(Benzylthio)pyrimidine (3ca). White solid. 55 – 56 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 4.8 Hz, 2H), 7.43 (d, *J* = 7.2 Hz, 2H), 7.32 – 7.28 (m, 2H), 7.26 – 7.21 (m, 1H), 6.96 – 6.94 (m, 1H), 4.41 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.3, 137.5, 129.2, 128.6, 127.3, 116.7, 35.4. This compound was known: Ma, X.; Yu, L.; Su, C.; Yang, Y.; Li, H.; Xu, Q. *Adv. Synth.*

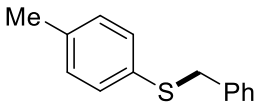
Catal. **2017**, *359*, 1649.



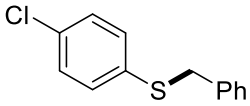
2-(Benzylthio)benzo[d]thiazole (3da). White solid. 38 – 39 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, J = 7.8 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.47 – 7.39 (m, 3H), 7.35 – 7.27 (m, 4H), 4.60 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.5, 153.2, 136.2, 135.4, 129.3, 128.8, 127.9, 126.2, 124.4, 121.6, 121.1, 37.8. This compound was known: Kumar, D.; Mishra, B. B.; Tiwari, V. K. *J. Org. Chem.* **2013**, *79*, 251.



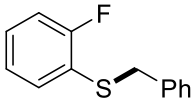
Benzyl(phenyl)sulfane (3ea). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 6H), 7.27 – 7.22 (m, 3H), 7.20 – 7.15 (m, 1H), 4.11 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 137.5, 136.4, 129.9, 128.9, 128.6, 127.3, 126.4, 39.1. This compound was known: Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.



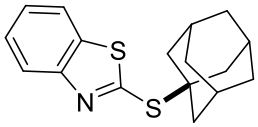
Benzyl(p-tolyl)sulfane (3fa). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 – 7.25 (m, 4H), 7.24 – 7.19 (m, 2H), 7.07 (d, J = 7.8 Hz, 2H), 4.07 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 137.9, 136.7, 132.5, 130.8, 129.7, 128.9, 128.5, 127.2, 39.9, 21.2. This compound was known: Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.



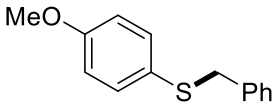
Benzyl(4-chlorophenyl)sulfane (3ga). White solid. 48 – 49 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 – 7.20 (m, 9H), 4.07 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 137.2, 134.7, 132.6, 131.5, 129.0, 128.9, 128.6, 127.4, 39.4. This compound was known: Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.



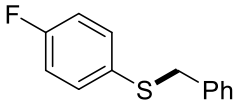
Benzyl(2-fluorophenyl)sulfane (3ha). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 – 6.99 (m, 9H), 4.09 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.8 (d, J = 245.2 Hz), 137.3, 133.1, 128.9, 128.9, 128.6, 127.3, 124.4 (d, *J* = 3.3 Hz), 122.8 (d, *J* = 17.9 Hz), 115.7 (d, *J* = 22.5 Hz), 38.5 (d, *J* = 2.0 Hz). This compound was known: Li, Y.; Pu, J.; Jiang, X. *Org. Lett.* **2014**, *16*, 2692.



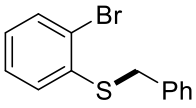
2-((1-adamantanyl)thio)benzo[d]thiazole (3dK). White solid. 120 – 121 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.38 (dd, *J* = 11.5, 4.1 Hz, 1H), 7.31 – 7.27 (m, 1H), 2.09 (d, *J* = 2.9 Hz, 6H), 2.02 (s, 3H), 1.63 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.9, 153.8, 137.1, 126.1, 125.1, 122.9, 121.0, 53.0, 43.6, 36.1, 30.3. IR (KBr): *v* 2917, 2849, 1735, 1467, 1371, 1236, 1020, 960, 720, 628, 608 cm^{-1}. HRMS (ESI) for $C_{17}H_{20}NS_2$ (M+H) Calcd: 301.0959; found: 301.0950.



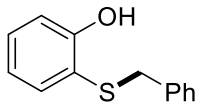
Benzyl(4-methoxyphenyl)sulfane (3ia). White solid. 48 – 49 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 – 7.15 (m, 7H), 6.84 – 6.74 (m, 2H), 3.98 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 138.2, 134.2, 129.0, 128.5, 127.1, 126.1, 114.5, 55.4, 41.3. This compound was known: Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.



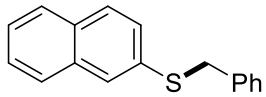
Benzyl(4-fluorophenyl)sulfane (3ja). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 – 7.19 (m, 7H), 6.96 – 6.90 (m, 2H), 4.02 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2 (d, *J* = 246.9 Hz), 137.6, 133.5 (d, *J* = 7.9 Hz), 130.8, 128.9, 128.6, 127.3, 116.0 (d, *J* = 21.7 Hz), 40.5. This compound was known: Reeves, J. T.; Camara, K.; Han, Z.; Xu, Y.; Lee, H.; Busacca, C.; Senanayake, C. H. *Org. Lett.* **2014**, *16*, 1196.



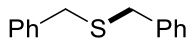
Benzyl(2-bromophenyl)sulfane (3ka). White solid. 49 – 50 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, J = 7.8 Hz, 1H), 7.36 (d, J = 7.2 Hz, 2H), 7.30 (dd, J = 7.2, 7.2 Hz, 2H), 7.28 – 7.19 (m, 3H), 7.08 – 6.97 (m, 1H), 4.15 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.0, 136.2, 133.0, 129.1, 128.9, 128.7, 127.8, 127.5, 127.0, 123.7, 38.0. This compound was known: Li, Y.; Pu, J.; Jiang, X. *Org. Lett.* **2014**, *16*, 2692.



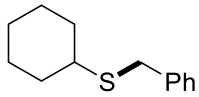
2-(Benzylthio)phenol (3la). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 – 7.22 (m, 5H), 7.10 – 7.02 (m, 2H), 6.92 (d, J = 7.8 Hz, 1H), 6.82 – 6.78 (m, 1H), 6.54 (d, J = 1.8 Hz, 1H), 3.84 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.2, 137.7, 136.5, 131.5, 128.9, 128.7, 127.5, 120.7, 118.3, 114.8, 41.5. This compound was known: Li, Y.; Pu, J.; Jiang, X. *Org. Lett.* **2014**, *16*, 2692.



Benzyl(naphthalen-2-yl)sulfane (3ma). White solid. 89 – 90 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, J = 7.8 Hz, 1H), 7.77 – 7.72 (m, 2H), 7.71 (d, J = 7.8 Hz, 1H), 7.49 – 7.39 (m, 3H), 7.34 (d, J = 7.2 Hz, 2H), 7.31 – 7.28 (m, 2H), 7.28 – 7.22 (m, 1H), 4.23 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 137.4, 134.0, 133.8, 132.0, 129.0, 128.7, 128.4, 127.8, 127.8, 127.7, 127.4, 127.3, 126.6, 125.8, 39.0. This compound was known: Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.



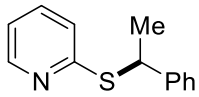
Dibenzylsulfane (3na). White solid. 48 – 49 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 – 7.14 (m, 10H), 3.60 (s, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.2, 129.1, 128.6, 127.1, 35.7. This compound was known: Y Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.



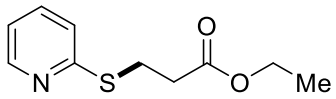
Benzyl(cyclohexyl)sulfane (3oa). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.20 (m, 5H), 3.73 (s, 2H), 2.59 – 2.52 (m, 1H), 2.01 – 1.90 (m, 2H), 1.77 – 1.70 (m, 2H), 1.41 – 1.10 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.0, 128.8, 128.5, 126.9, 43.0, 34.7, 33.5, 26.1, 26.0. This

compound was known: Yang, Y.; Ye, Z.; Zhang, X.; Zhou, Y.; Ma, X.; Cao, H.; Li, H.; Yu, L.; Xu, Q. *Org. Biomol. Chem.* **2017**, *15*, 9638.

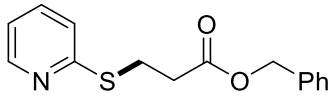
Typical procedure for the acid-catalyzed addition reactions of disulfide with alkenens or alkynes. The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol), styrene **5a** (52.0 mg, 0.50 mmol, 1.0 equiv.), water (45.0 mg, 2.5 mmol, 5.0 equiv.) and $TsOH{\cdot}H_2O$ (95.0 mg, 0.50 mmol, 100 mol%) was sealed in a Schlenk tube (10 mL) under nitrogen and stirred at 130 ^oC for 12 h. The reaction mixture was then analyzed by TLC/GC-MS and purified by flash column chromatography on silica gel using ethyl acetate and petroleum ether (0~ 1/20) as the eluent, giving **6a** in 45% isolated yield.



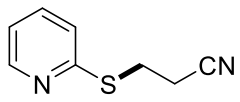
2-((1-Phenylethyl)thio)pyridine (6a). Yellow oil. ^1H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 4.8 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.30 (dd, J = 7.2, 7.2 Hz, 2H), 7.22 (dd, J = 7.2, 7.2 Hz, 1H), 7.10 (d, J = 7.8 Hz, 1H), 6.96 (dd, J = 6.6, 5.4 Hz 1H), 5.10 (q, J = 7.2 Hz, 1H), 1.74 (d, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.9, 149.6, 143.4, 136.1, 128.6, 127.5, 127.2, 122.9, 119.7, 43.7, 22.7. This compound was known: Ma, H.; Ren, X.; Zhou, X.; Ma, C.; He, Y.; Huang, G. *Tetrahedron Lett.* **2015**, *56*, 6022.



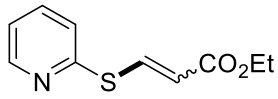
Ethyl 3-(pyridin-2-ylthio)propanoate (6c). Colorless oil. ^1H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, J = 4.2 Hz, 1H), 7.45 – 7.42 (m, 1H), 7.13 (d, J = 8.4 Hz, 1H), 6.99 – 6.89 (m, 1H), 4.13 (q, J = 7.2 Hz, 2H), 3.40 (t, J = 7.2 Hz, 2H), 2.74 (t, J = 7.2 Hz, 2H), 1.23 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.2, 158.3, 149.5, 136.0, 122.4, 119.5, 60.7, 34.8, 25.0, 14.3. This compound was known: Gholinejad, M.; Firouzabadi, H. *New J. Chem.* **2015**, *39*, 5953.



Benzyl 3-(pyridin-2-ylthio)propanoate (6d). Colorless oil. ^1H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, J = 4.8 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.37 – 7.29 (m, 5H), 7.14 (d, J = 7.8 Hz, 1H), 6.96 – 6.94 (m, 1H), 5.14 (s, 2H), 3.45 (t, J = 7.2 Hz, 2H), 2.84 (t, J = 7.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.1, 158.2, 149.6, 136.0, 135.9, 128.7, 128.3, 122.5, 119.6, 66.6, 34.8, 25.0. IR (KBr): ν 3034, 2997, 2939, 2854, 1731, 1578, 1556, 1454, 1414, 1124, 907, 756, 725, 696 cm^{-1}. HRMS (ESI) for $C_{15}H_{16}NO_2S$ (M+H) Calcd: 274.0902; found: 274.0891.



3-(Pyridin-2-ylthio)propanenitrile (6e). Colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, J = 4.2 Hz, 1H), 7.54 – 7.46 (m, 1H), 7.17 (d, J = 8.4 Hz, 1H), 7.05 – 6.97 (m, 1H), 3.40 (t, J = 7.2 Hz, 2H), 2.85 (t, J = 7.2 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.7, 149.7, 136.4, 122.8, 120.1 118.7, 25.6, 18.8. This compound was known: Gholinejad, M.; Firouzabadi, H. *New J. Chem.* **2015**, *39*, 5953.

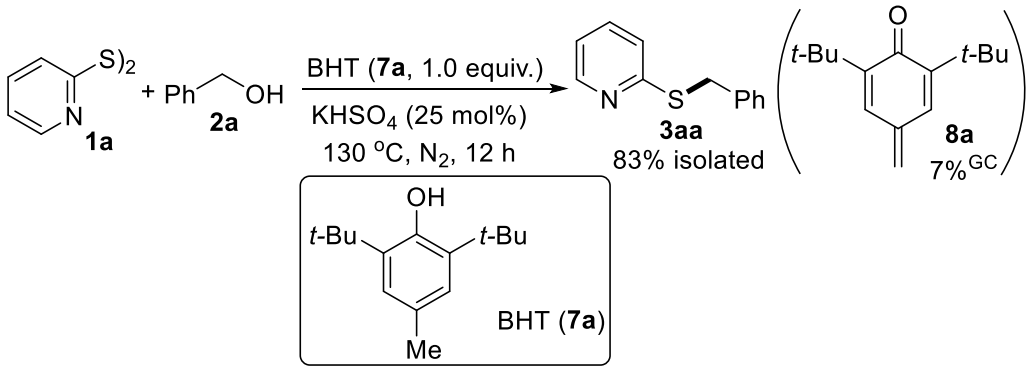


Ethyl 3-(pyridin-2-ylthio)acrylate (6f). Colorless oil. *Z* isomer: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, J = 10.2 Hz, 1H), 8.49 (d, J = 4.8 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 7.10 – 7.08 (m, 1H), 6.06 (d, J = 10.2 Hz), 4.22 (q, J = 7.8 Hz, 2H), 1.30 (t, J = 7.8 Hz, 3H); *E* isomer: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.54 (d, J = 16.2 Hz, 1H), 8.51 (d, J = 4.8 Hz, 1H), 7.60 – 7.58 (m, 1H), 7.24 (d, J = 8.4 Hz, 1H), 7.13 – 7.10 (m, 1H), 6.11 (d, J = 16.2 Hz, 1H), 4.20 (q, J = 14.4 Hz, 2H), 1.28 (t, J = 7.8 Hz, 3H); *Z* isomer: ^{13}C NMR (150 MHz, $CDCl_3$) δ 116.9, 155.3, 149.7, 142.0, 136.9, 123.4, 121.4, 114.0, 60.5, 14.4; *E* isomer: ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.3, 154.3, 150.2, 141.9, 137.0, 123.3, 121.6, 117.4, 60.5, 14.4. This compound was known: Kabir, M. S.; Lorenz, M.; Linn, M. L. V.; Namjoshi, O. A.; Ara, S.; Cook, J. M. *J. Org. Chem.* **2010**, *75*, 3626.

3. Control Reactions for Mechanistic Studies

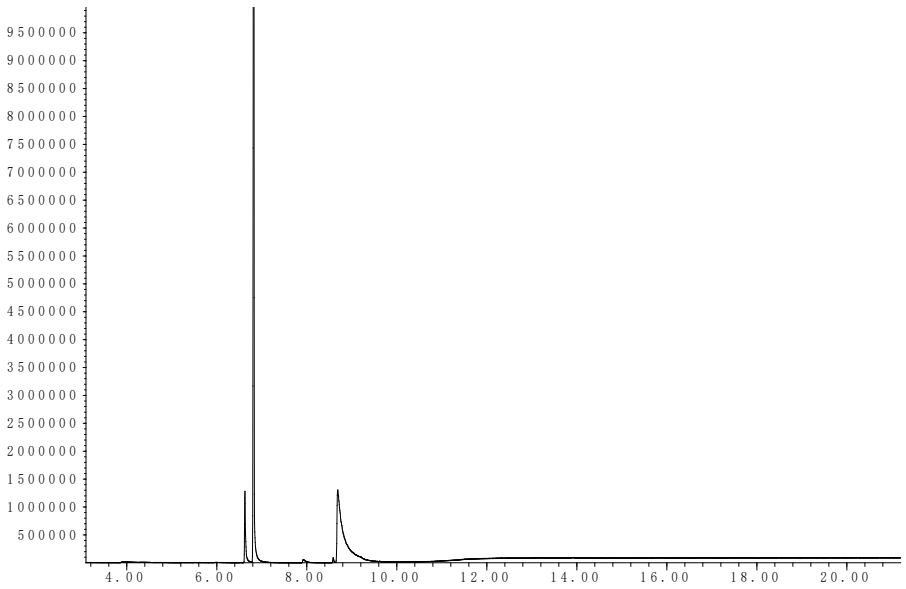
3.1 Studies on the possibilities of S-S bond cleavage

3.1.1 The reaction of 1a and 2a using BHT (7a) as the radical trapping reagent (eq. 1 in the main text)



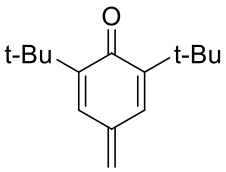
Detailed Procedure: The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol), benzyl alcohol **2a** (54.0 mg, 0.50 mmol), $KHSO_4$ (17.0 mg, 0.125 mmol, 25 mol%), and BHT **7a** (110.0 mg, 0.50 mmol, 1.0 equiv.) was directly sealed in a Schlenk tube (10 mL) under nitrogen, and then stirred at 130 ^oC for 12 h. The reaction mixture was analyzed by TLC/GC-MS, and then purified by flash column chromatography on silica gel using ethyl acetate and petroleum ether (0~ 1/50) as the eluent, giving **3aa** in 83% isolated yield.

GC Spectra

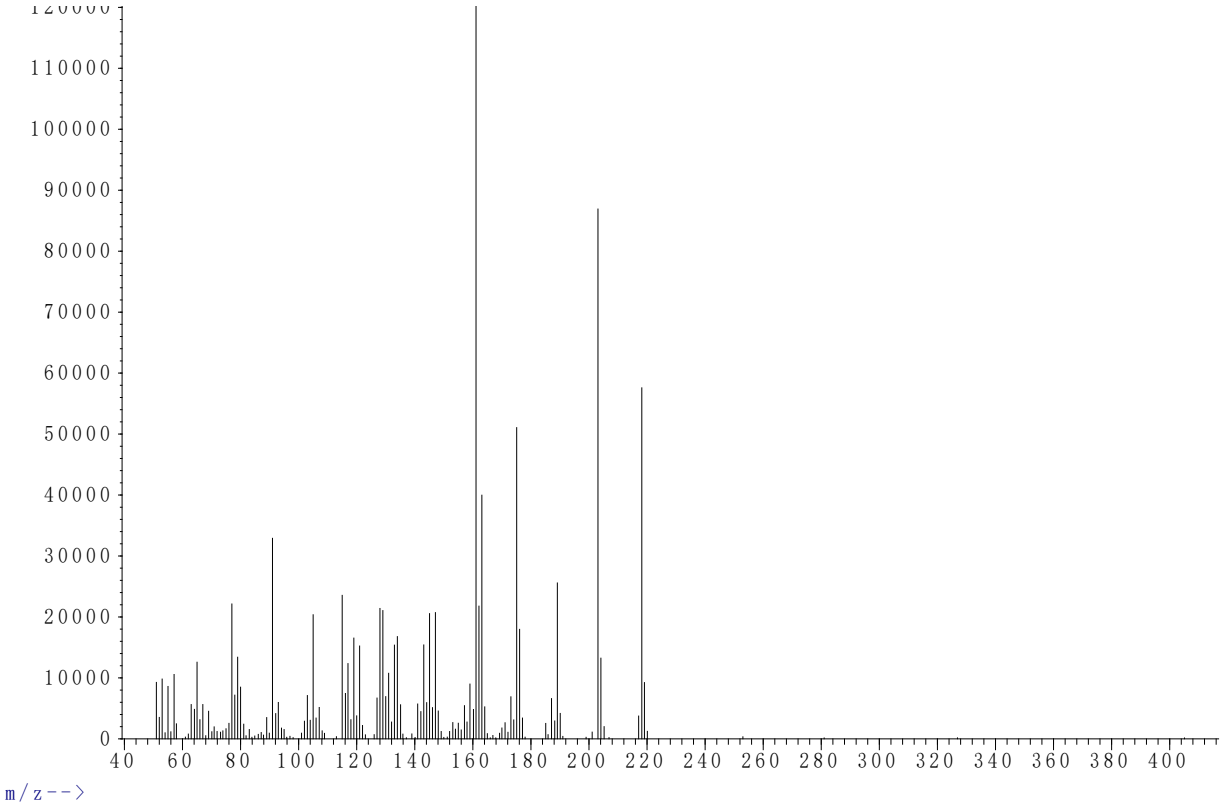


Run	Time /min	Start scanning	Peak scanning	Stop scanning	Peak type	Hight	Correction area	Correction maximum%	Total%
1	6.629	755	760	778	M	1283166	19880827	8.01	**7.415**
2	6.820	791	802	829	M	20587982	248230085	100.00	**92.585**

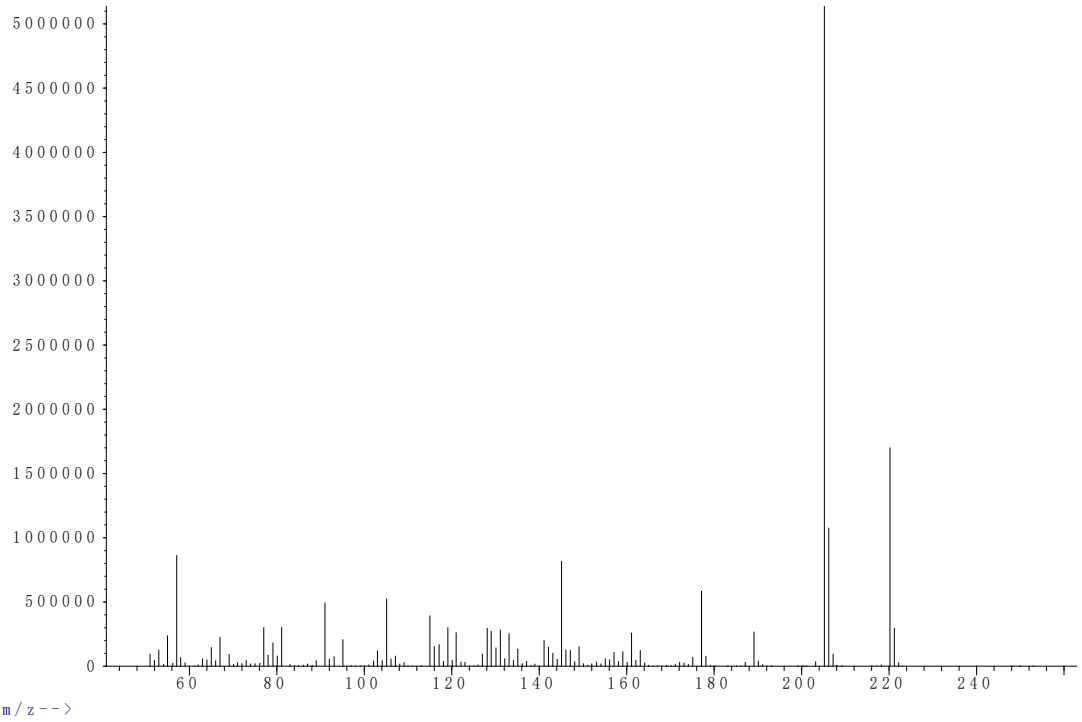
MS Spectra



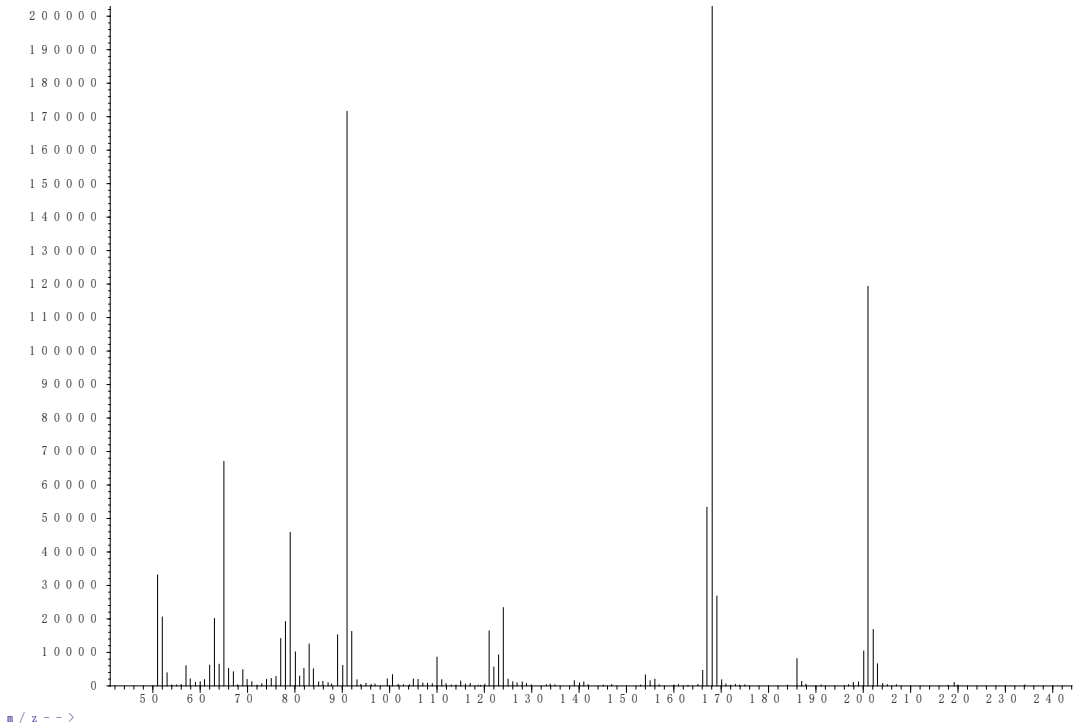
T = 6.629 min, m/z =218, (**8a**)



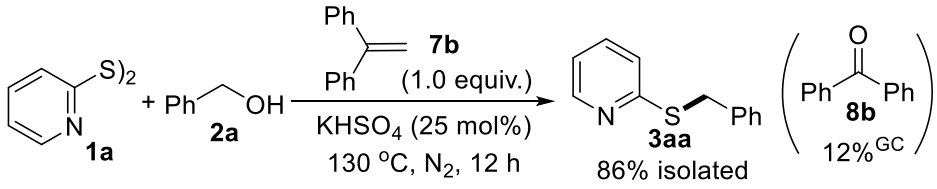
T = 6.820 min, m/z =220, BHT (**7a)**



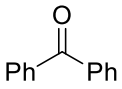
T = 8.751 min, m/z = 201, (**3aa**)



3.1.2 The reaction of 1a and 2a using 1,1-diphenylethene (7b) as the radical trapping reagent (eq. 2 in the main text)

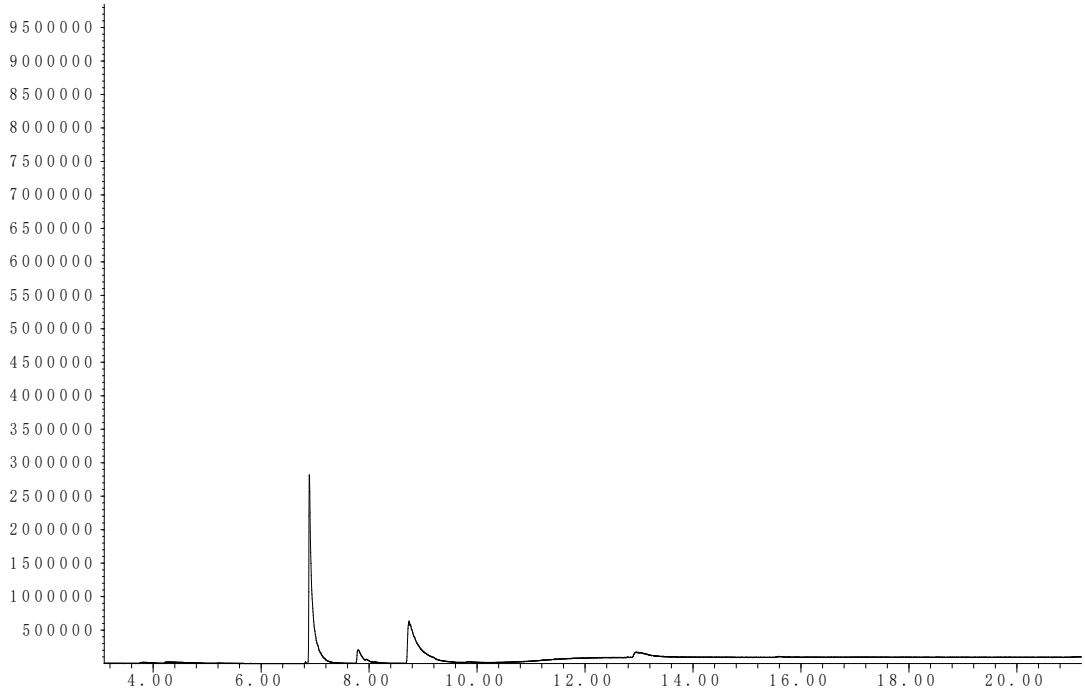


Detailed Procedure: The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol), benzyl alcohol **2a** (54.0 mg, 0.50 mmol), $KHSO_4$ (17.0 mg, 0.125 mmol, 25 mol%), and 1,1-diphenylethene **7b** (90.0 mg, 0.50 mmol, 1.0 equiv.) was directly sealed in a Schlenk tube (10 mL) under nitrogen, and then stirred at 130 ^oC for 12 h. The reaction mixture was analyzed by TLC/GC-MS, and then purified by flash column chromatography on silica gel using ethyl acetate and petroleum ether (0~ 1/50) as the eluent, giving **3aa** in 86% isolated yield.



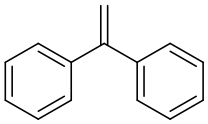
Benzophenone (8b). White solid. 48 – 49 ^oC. ^1H NMR (600 MHz, $CDCl_3$) δ 7.85 – 7.74 (m, 4H), 7.62 – 7.55 (m, 2H), 7.50 – 7.44 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.9, 137.7, 132.5, 130.2, 128.4. This compound was known: Yang, X.-J.; Zheng, Y.-W.; Zheng, L.-Q.; Wu, L.-Z.; Tung, C.-H.; Chen, B. *Green Chem.* **2019**, *21*, 1401.

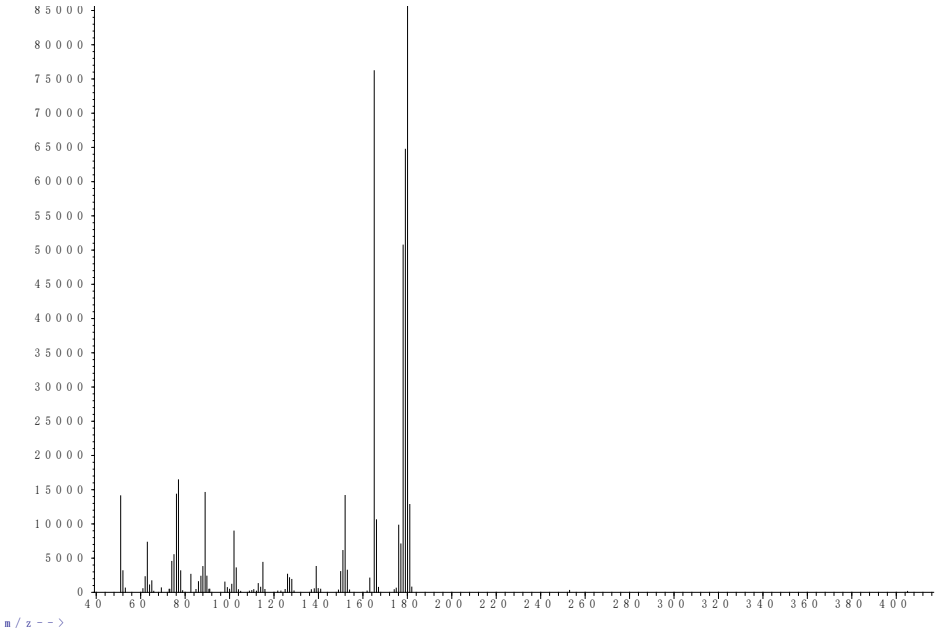
GC Spectra

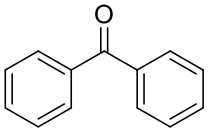


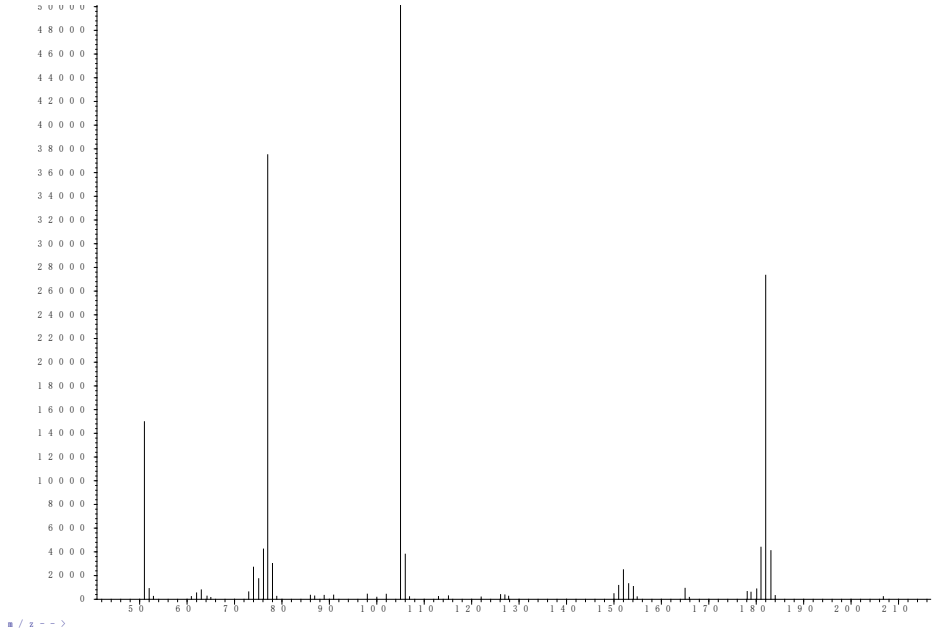
Run	Time /min	Start scanning	Peak scanning	Stop scanning	Peak type	Hight	Correction area	Correction maximum%	Total%
1	6.993	811	818	899	M	2846164	118361192	100.00	**88.137**
2	7.821	1001	1013	1072	M2	201943	15931163	13.46	**11.863**

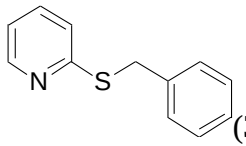
MS Spectra

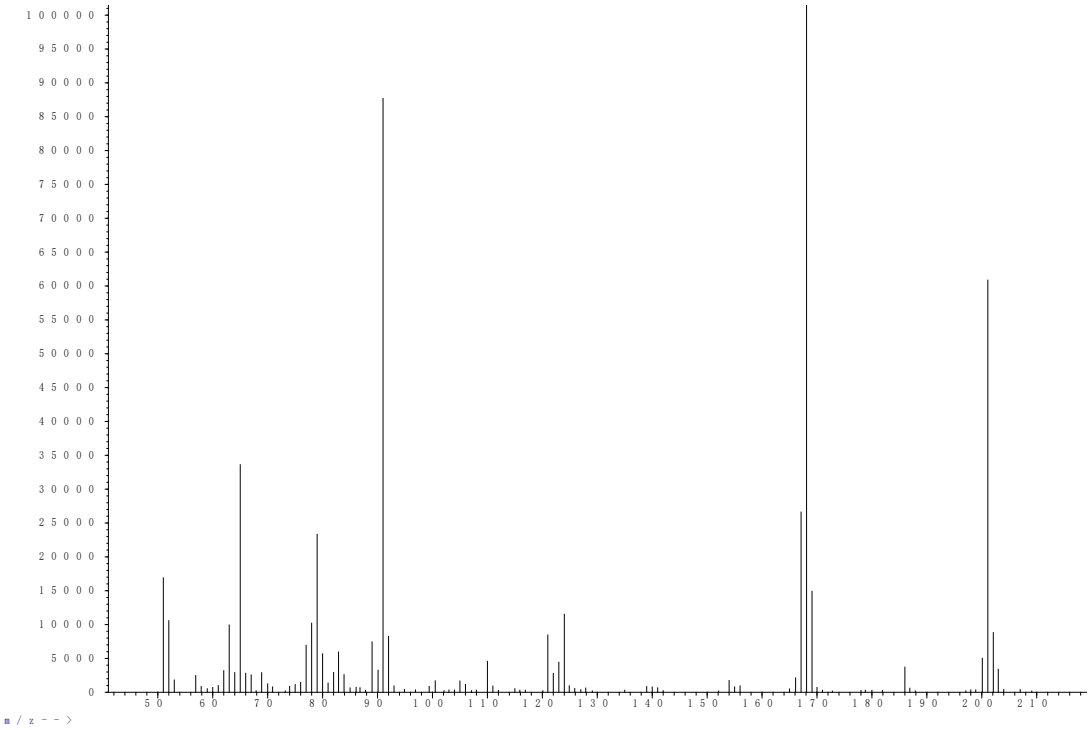
T = 6.993 min, m/z = 180,  (**7b**)



T = 7.821 min, m/z = 182,  (**8b**)



T = 8.776 min, m/z = 201,  (**3aa**)



3.1.3 Results and Discussion

When 3,5-di-*t*-butyl 4-hydroxyl toluene (BHT, **7a**) or 1,1-diphenylethene (**7b**) was added to the model reaction of **1a** and **2a**, the target product **3aa** could still be obtained in good yields. Therefore, the reaction should not proceed via the formation of radical intermediates by homolytic cleavage of the S-S bond, but more likely the heterolytic cleavage of the S-S bond to give thiol cation (RS^+) and thiol (RSH) intermediates in the presence of the acid catalyst. Besides, certain amounts of 2,6-di-*tert*-butyl-4-methylenecyclohexa-2,5-dien-1-one (**8a**) and benzophenone (**8b**), the oxidation products of **7a** and **7b**, were also observed by GC-MS analysis of these reactions. This may indicate that, certain oxidizing species may be generated in the reaction that can oxidize **7a** and **7b** to **8a** and **8b**.

3.2 Determination of possible intermediates by isotope labeling experiments

3.2.1 Certificate of analysis of the purchased $H_2{}^{18}O$ (98 atom% ^{18}O)

CERTIFICATE OF ANALYSIS

Catalog No.	:	204174	Lot Number	: LN30U38
Product Name	:	Water-^{18}O, N/A, 90 atom%^{18}O		
CAS	:	14314-42-2		
Version	:	1.2		
Molecular Formula	:	$H_2{}^{18}O$		
Molecular Weight	:	20.02	Issue Date : 2020-03-23	

Appearance	:	Clear colorless liquid
Assay	:	98.32 atom % 18O

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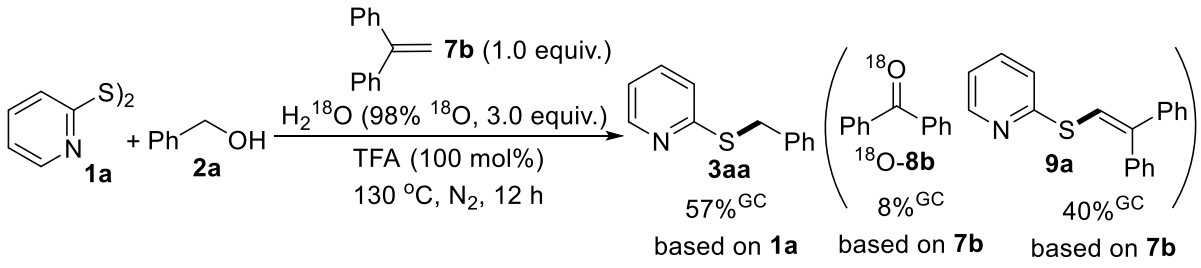
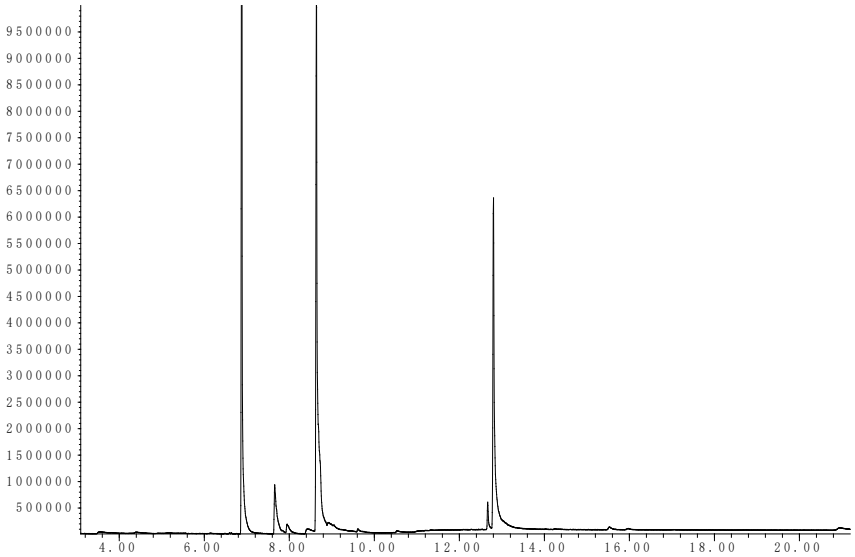
3.2.2 The reaction of 1a, 2a and 7b in the presence of ^{18}O-H_2O (98 atom% ^{18}O) (eq. 3 in the main text)



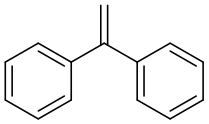
Detailed Procedure: The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol), benzyl alcohol **2a** (54.0 mg, 0.50 mmol), 1,1-diphenylethene **7b** (90.0 mg, 0.50 mmol, 1.0 equiv.), TFA (57.0 mg, 0.50 mmol, 1.0 equiv.), and $H_2{}^{18}O$ (98 atom% ^{18}O, 27.0 mg, 1.5 mmol, 3.0 equiv.) was directly sealed in a Schlenk tube (10 mL) under nitrogen, and then stirred at 130 ^{o}C for 12 h. The reaction mixture was then analyzed by GC-MS.

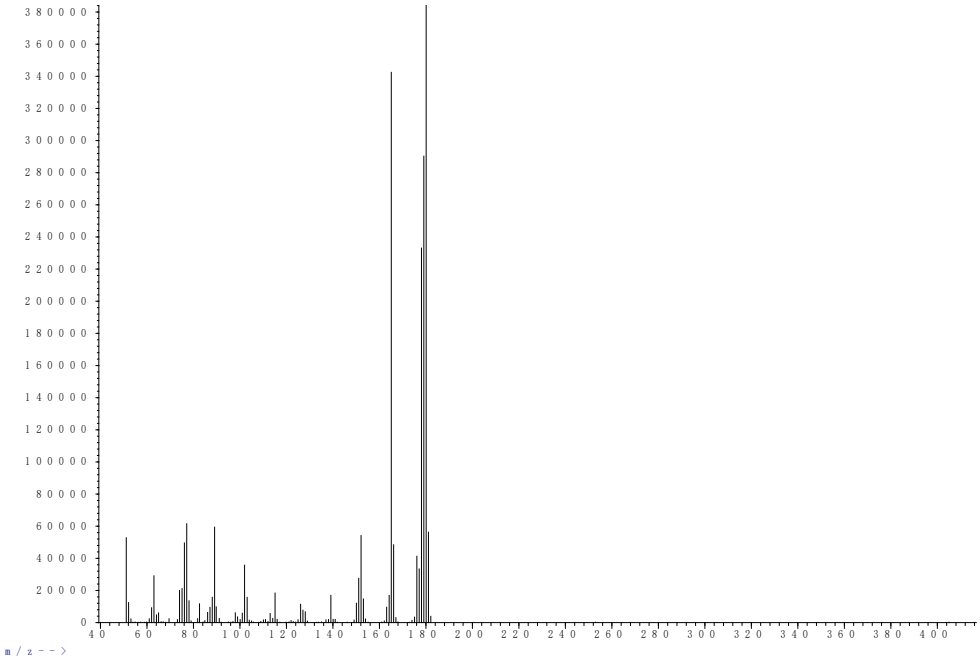
GC Spectra

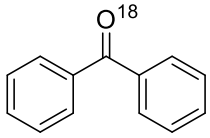


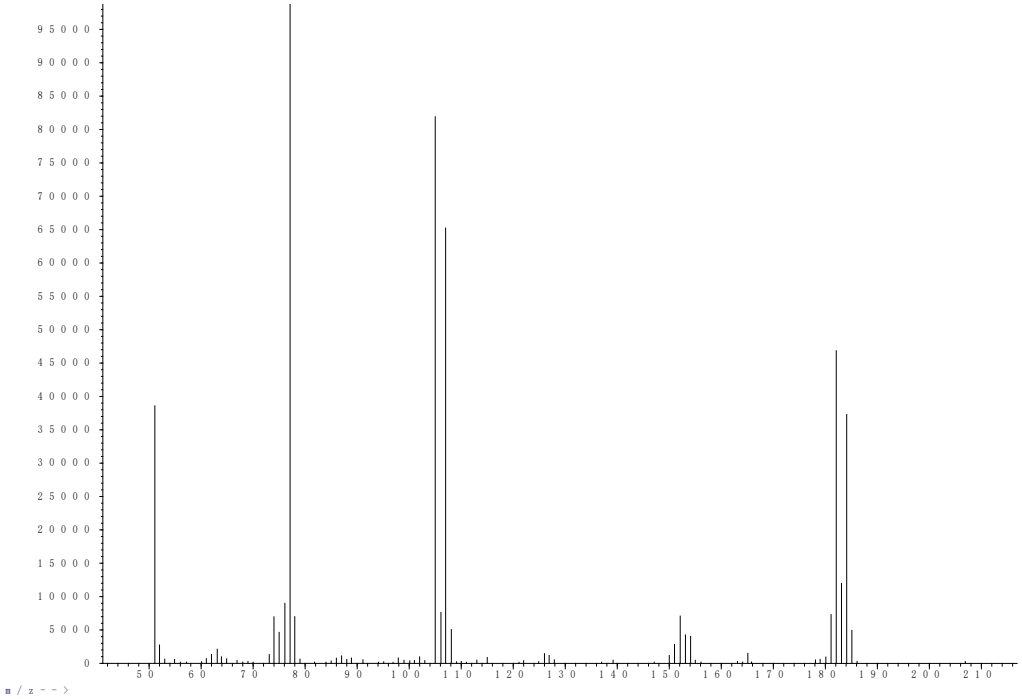
Run	Time /min	Start scanning	Peak scanning	Stop scanning	Peak type	Hight	Correction area	Correction maximum%	Total%
1	6.899	802	815	866	M	17887132	260324586	100.00	**52.156**
2	7.695	967	981	1020	M	942556	39770227	15.28	**7.968**
3	12.830	2073	2087	2235	M	6320215	199032156	76.46	**39.876**

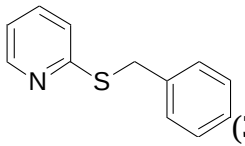
MS Spectra

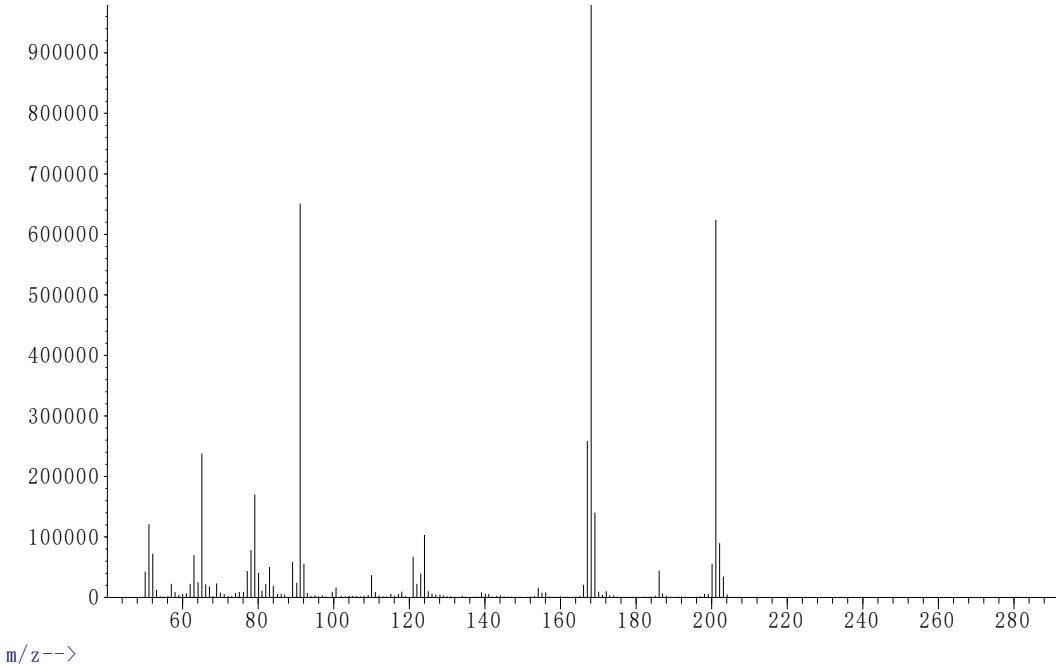
T = 6.899 min, m/z =180,  (**7b**)

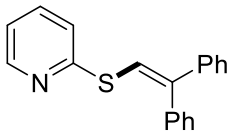


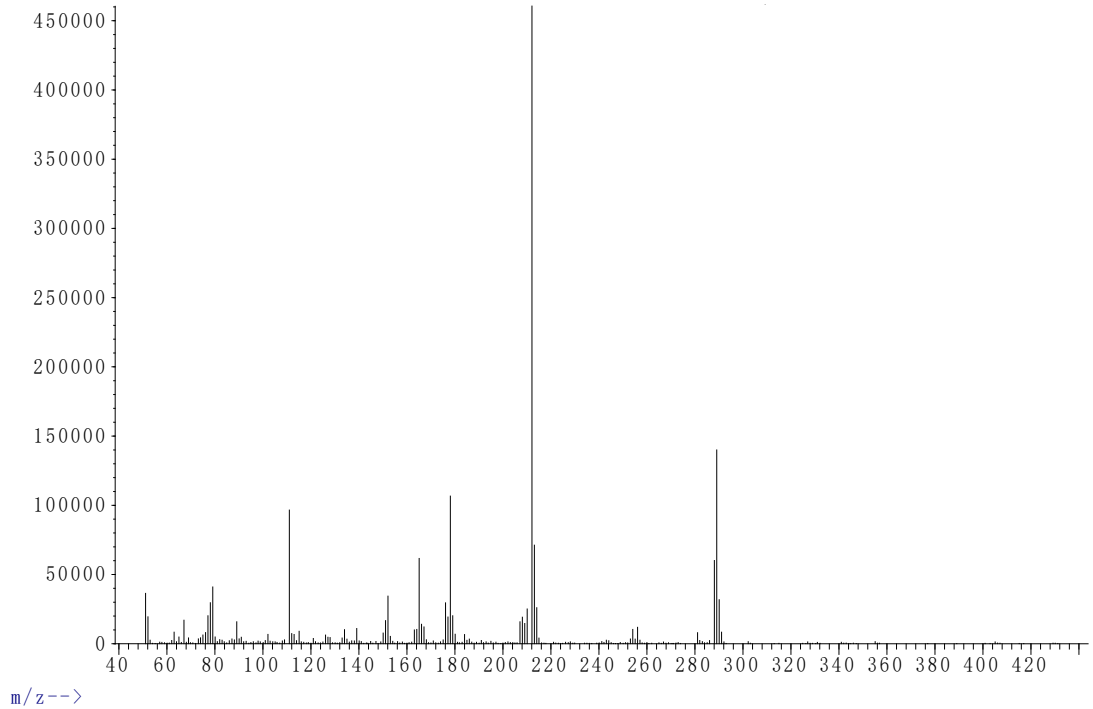
T = 7.695 min, m/z = 184,  (**^{18}O-8b**)



T = 8.650 min, m/z = 201,  (**3aa**)

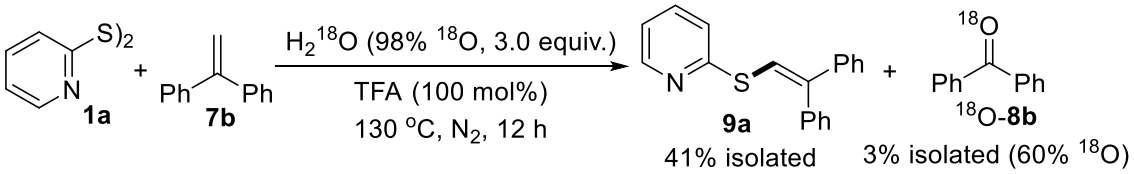


T = 12.830 min, m/z = 289,  (**9a**)



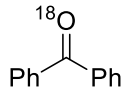
Results and Discussion: The observed **9a** should be generated by an electrophilic reaction of 2-pyridylthiol cation 2-PyS^+ (**10a**) with alkene **7b**, implying that the reaction should proceed *via* the formation of 2-PyS^+ (**10a**) and RSH intermediates by heterolytic cleavage of S-S bond of **1a**. Besides, ^{18}O-**8b** that may be generated from the oxidation of **7b** was also detected by GC-MS, suggesting that certain oxidizing species (containing ^{18}O) was generated from ^{18}O-H_2O in the reaction.

3.2.3 The reaction of 1a and 7b in the presence of ^{18}O-H_2O (98% ^{18}O) (eq. 4 in the main text)

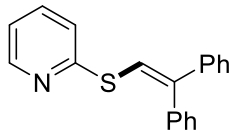


Detailed Procedure: The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol), 1,1-diphenylethene **7b** (90.0 mg, 0.50 mmol, 1.0 equiv.), TFA (57.0 mg, 0.50 mmol, 1.0 equiv.), and $H_2{}^{18}O$ (98 atom % ^{18}O, 27.0 mg, 1.5 mmol, 3.0 equiv.) was directly sealed in a Schlenk tube (10 mL) under nitrogen, and stirred at 130 ^oC for 12 h. The reaction mixture was then analyzed by GC-MS and purified by flash column chromatography on silica gel using ethyl acetate and petroleum ether (0~ 1/20) as the eluent, giving **9a** and **^{18}O-8b** in 41% and 3% isolated yield, respectively. Then the isotope analysis of the product **^{18}O-8b** by HRMS showed that ^{18}O-**8b**

should contain 60 atom% ^{18}O.

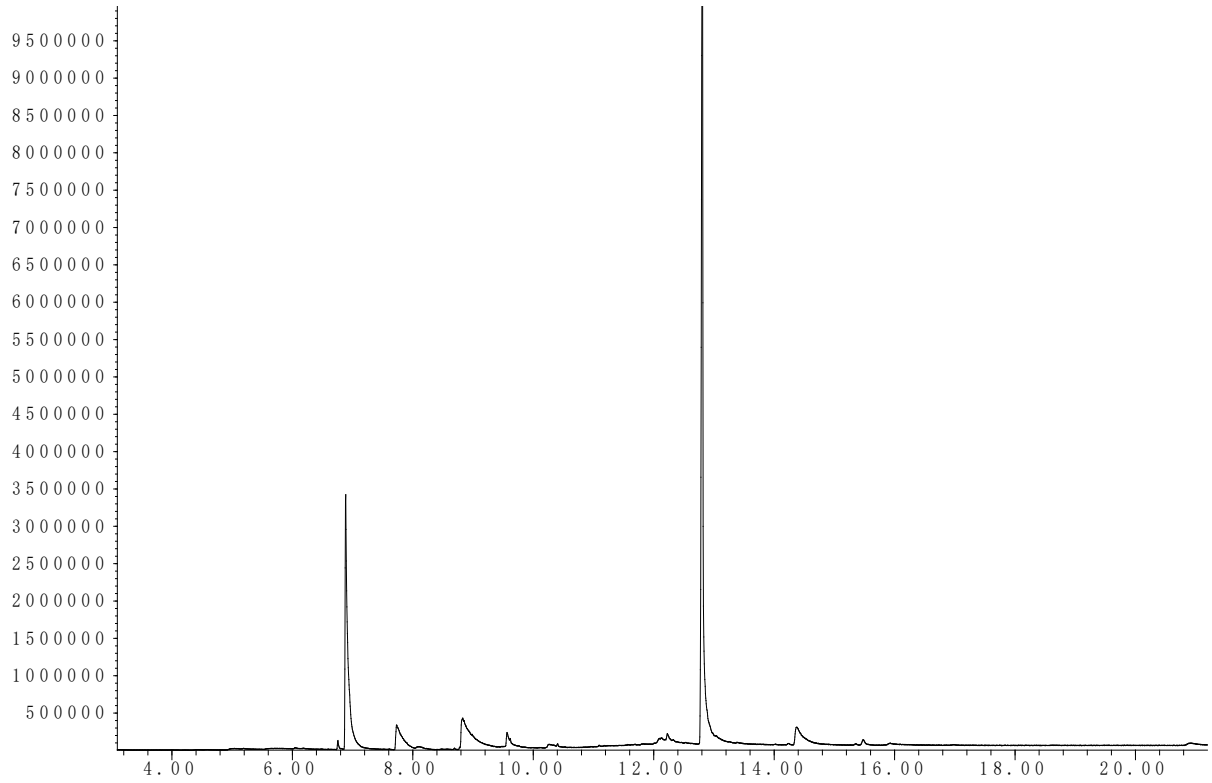


Benzophenone (^{18}O-8b). White solid. 48 – 49 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 – 7.77 (m, 4H), 7.62 – 7.55 (m, 2H), 7.52 –7.46 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.9, 137.7, 132.5, 130.2, 128.4. HRMS (EI) for $C_{13}H_{10}{}^{18}O$ (M) Calcd: 184.0774; found: 184.0772.



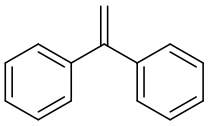
2-((2,2-Diphenylvinyl)thio)pyridine (9a). Colorless oil**.** ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.50 (dd, *J* = 4.8, 1.8 Hz, 1H), 7.75 (s, 1H), 7.52 – 7.48 (m, 1H), 7.42 (dd, *J* = 8.4, 6.0 Hz, 2H), 7.40 – 7.32 (m, 2H), 7.36 – 7.30 (m, 3H), 7.30 (dd, *J* = 8.4, 6.6 Hz, 2H), 7.26 – 7.24 (m, 1H), 7.19 – 7.17 (m, 1H), 7.06 – 7.03 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.3, 149.8, 141.5, 140.4, 139.9, 136.5, 129.8, 128.6, 128.4, 127.9, 127.4, 122.6, 120.4, 119.6. HRMS (ESI) for $C_{19}H_{16}NS$ (M+H) Calcd: 290.1003; found: 290.1031. Chen, Y.; Wen, S.; Tian, Q.; Zhang, Y.; Cheng, G. *Org. Lett.* **2021**, *23*, 7905.

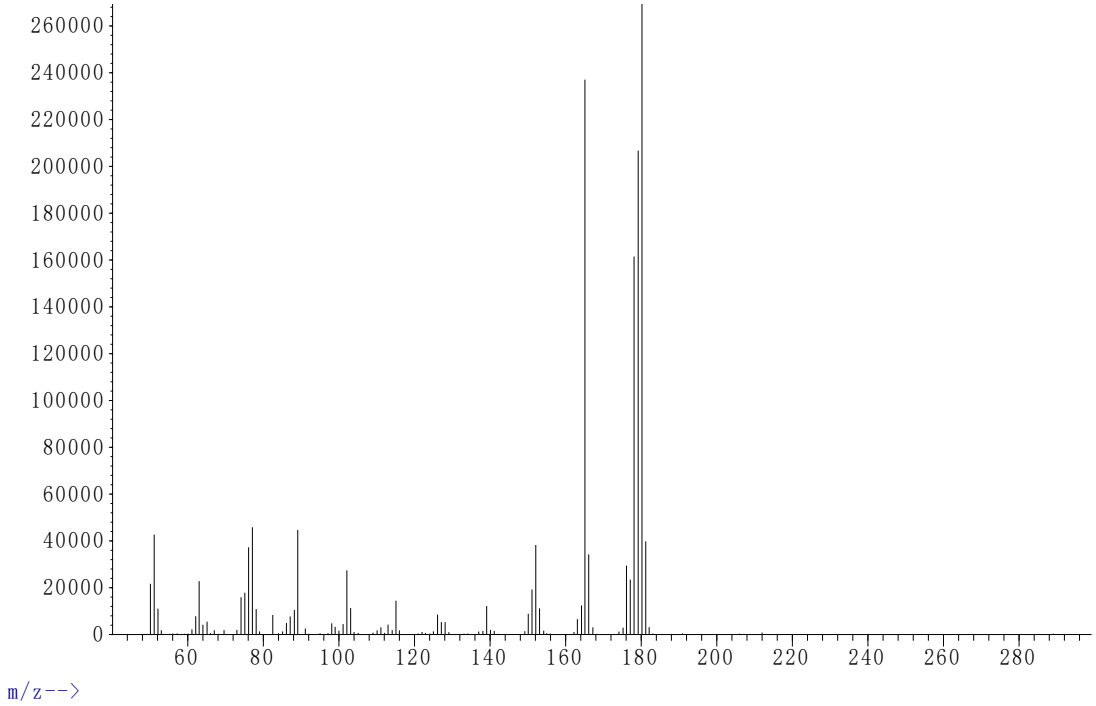
GC Spectra

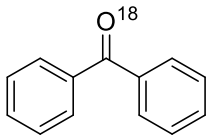


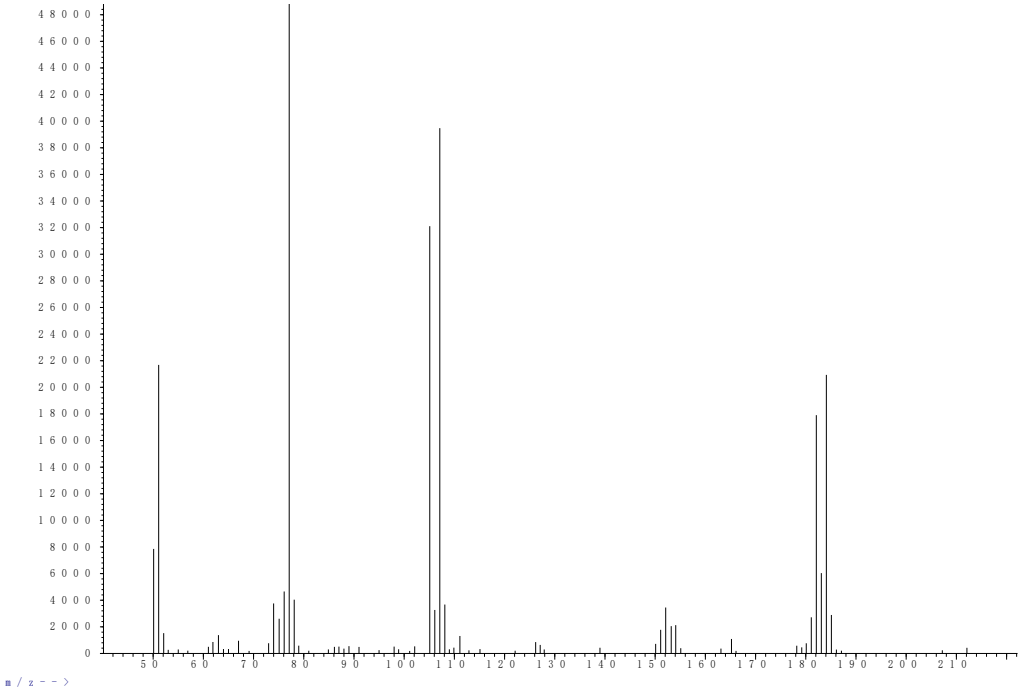
Run	Time /min	Start scanning	Peak scanning	Stop scanning	Peak type	Hight	Correction area	Correction maximum%	Total%
1	6.914	805	817	859	M	27958514	430645500	65.24	**38.211**
2	7.776	963	982	1020	M	786300	36222224	5.49	**3.214**
3	12.849	2063	2096	2131	M	21851283	660138794	100.00	**39.876**

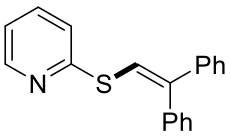
MS Spectra

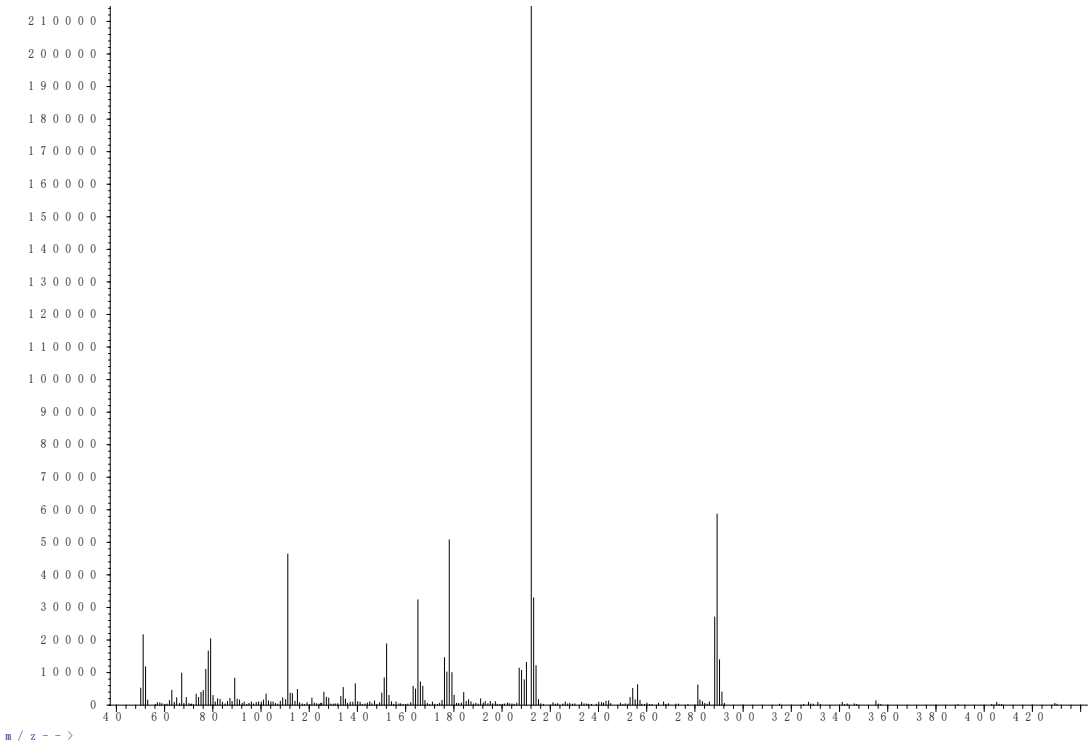
T = 6.914 min, m/z =180,  (**7b**)



T = 7.776 min, m/z = 184,  (**^{18}O-8b**)



T = 12.849 min, m/z = 289,  (**9a**)

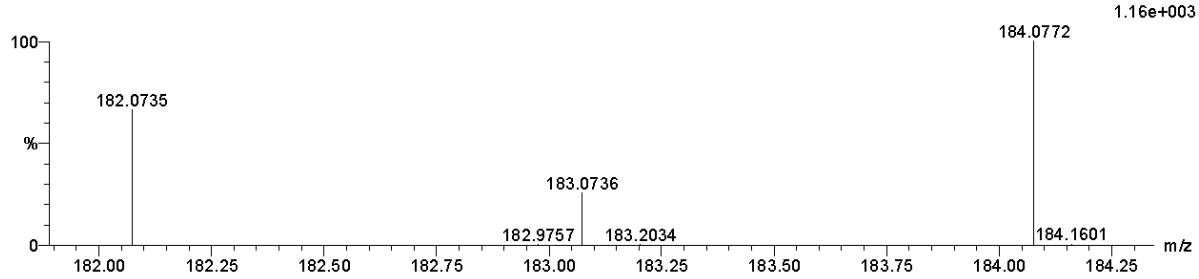


Isotope analysis of the obtained ^{18}O-8b by HRMS

Elemental Composition Report Page 1

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

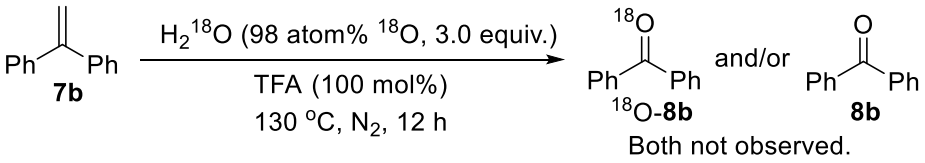
Monoisotopic Mass, Odd and Even Electron Ions
156 formula(e) evaluated with 2 results within limits (up to 70 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-100 16O: 0-5 18O: 0-5
CXK-1 460 (2.639)
TOF MS EI+



Minimum:	30.00				-1.5		
Maximum:	100.00		1.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
182.0735	66.35	182.0732	0.3	1.6	9.0	623.4	C13 H10 160
184.0772	100.00	184.0774	-0.2	-1.1	9.0	2773464.3	C13 H10 180

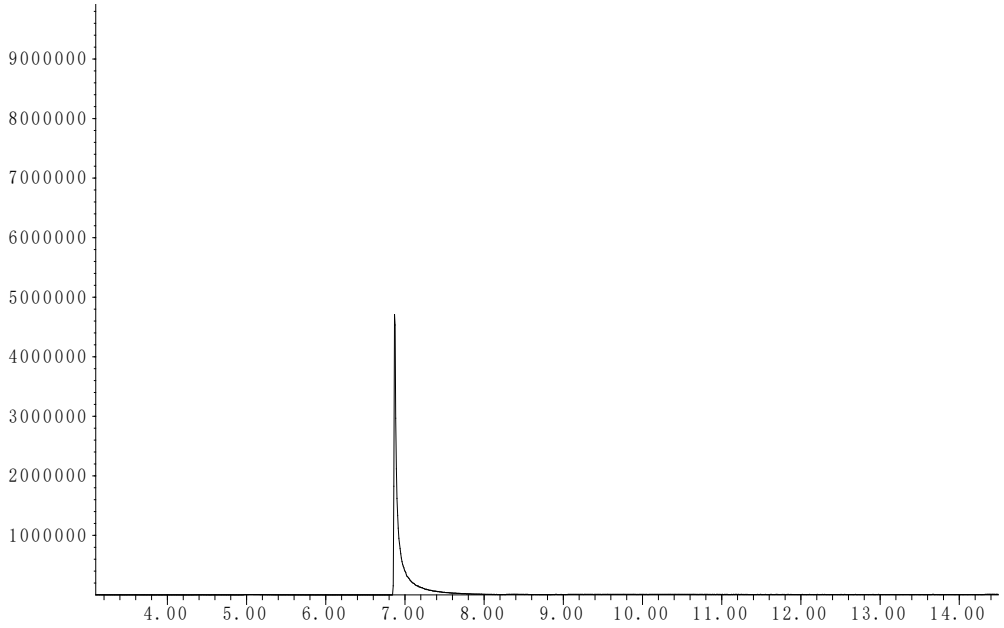
Results and Discussion: Observation of **9a** in the reaction confirmed again the possibility of heterolytic cleavage of **1a** to generate 2-PyS$^+$ (**10a**) under the acid-catalyzed conditions. Moreover, ^{18}O-**8b** was detected, isolated and determined to be containing 60 atom% ^{18}O by HRMS analysis, suggesting that certain oxidizing species (containing ^{18}O, possibly $H_2{}^{18}O_2$) may be generated from the reaction of ^{18}O-H_2O with **1a** or 2-PyS$^+$ (**10a**), but more possibly **10a** because no reaction can occur without the acid catalyst.

3.2.4 Control reaction of lone 7b with ^{18}O-H_2O (eq. 5 in the main text)



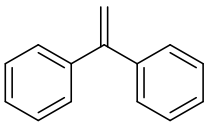
Detailed Procedure: The mixture of 1,1-diphenylethene **7b** (90.0 mg, 0.50 mmol, 1.0 equiv.), TFA (57.0 mg, 0.50 mmol, 1.0 equiv.), and $H_2{}^{18}O$ (98 atom% ^{18}O, 27.0 mg, 1.5 mmol, 3.0 equiv.) was directly sealed in a Schlenk tube (1 mL) under nitrogen, and then stirred at 130 ^{o}C for 12 h. The reaction mixture was analyzed by GC-MS, showing no **8b** was produced.

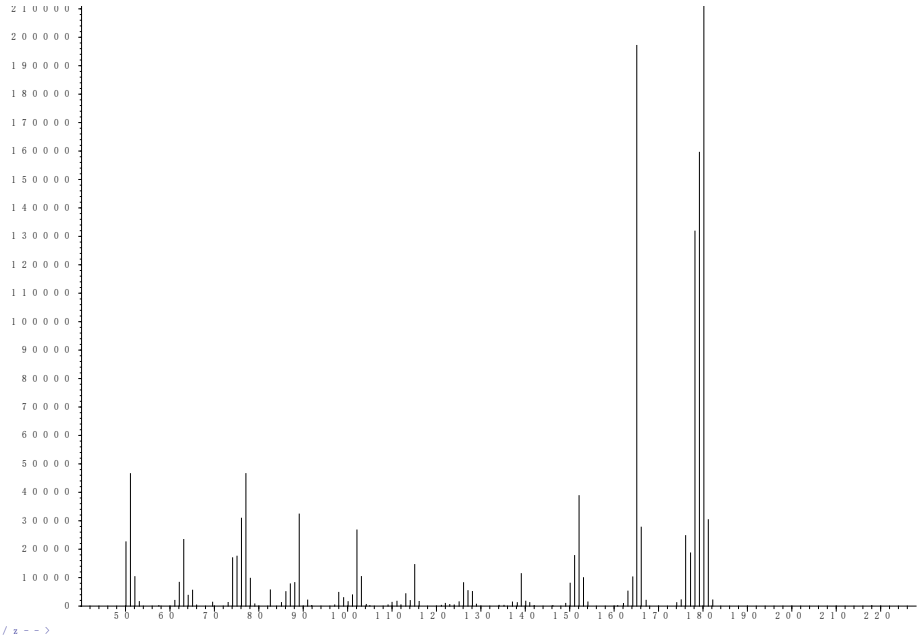
GC Spectra



Run	Time /min	Start scanning	Peak scanning	Stop scanning	Peak type	Hight	Correction area	Correction maximum%	Total%
1	6.871	475	478	512	M	5006000	148767287	100.00	**100.000**

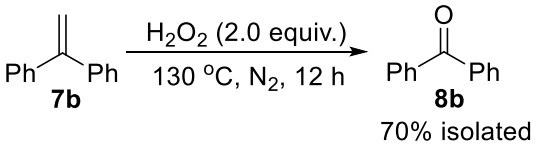
MS Spectra

T = 6.907 min, m/z =180,  (**7b**)



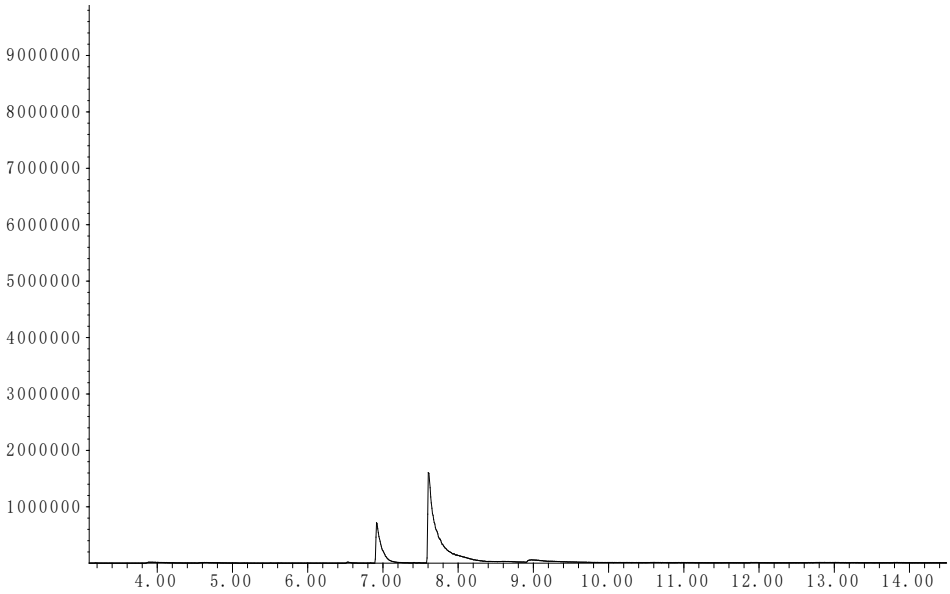
Results and Discussion: In the absence of **1a**, 1,1-diphenylethene **7b** cannot be oxidized to **8b**. Therefore, under the **1a**-free conditions, the potential oxidizing species (containing ^{18}O, possibly hydrogen peroxide $H_2{}^{18}O_2$) could not be generated from ^{18}O-H_2O. Ultimately, no **8b** could be generated from **7a**.

3.2.5 Control reaction of 1,1-diphenylethene (7b) with external H_2O_2 (eq. 6 in the main text)



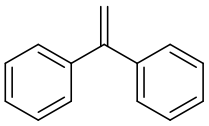
Detailed Procedure: The mixture of 1,1-diphenylethene **7b** (90.0 mg, 0.50 mmol, 1.0 equiv.) and H_2O_2 (100 mg, 1.0 mmol, 30 W/W%, 2.0 equiv.) was directly sealed in a Schlenk tube (1 mL) under nitrogen, and then stirred at 130 ^oC for 12 h. The reaction mixture was analyzed by GC-MS and purified by flash column chromatography on silica gel using ethyl acetate and petroleum ether (0~ 1/20) as the eluent, giving **8b** in 70% isolated yield.

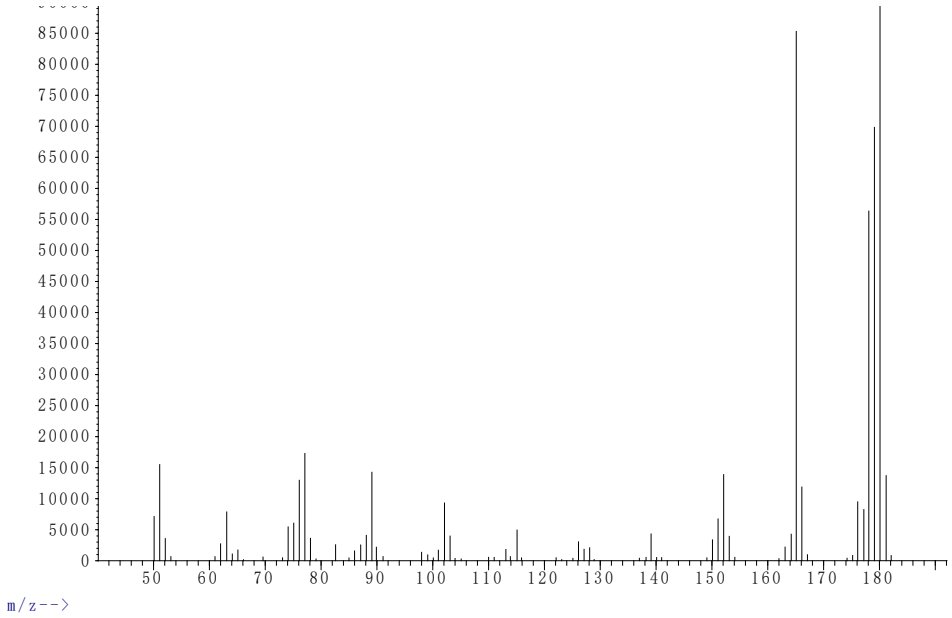
GC Spectra

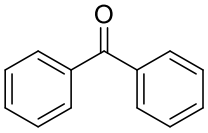


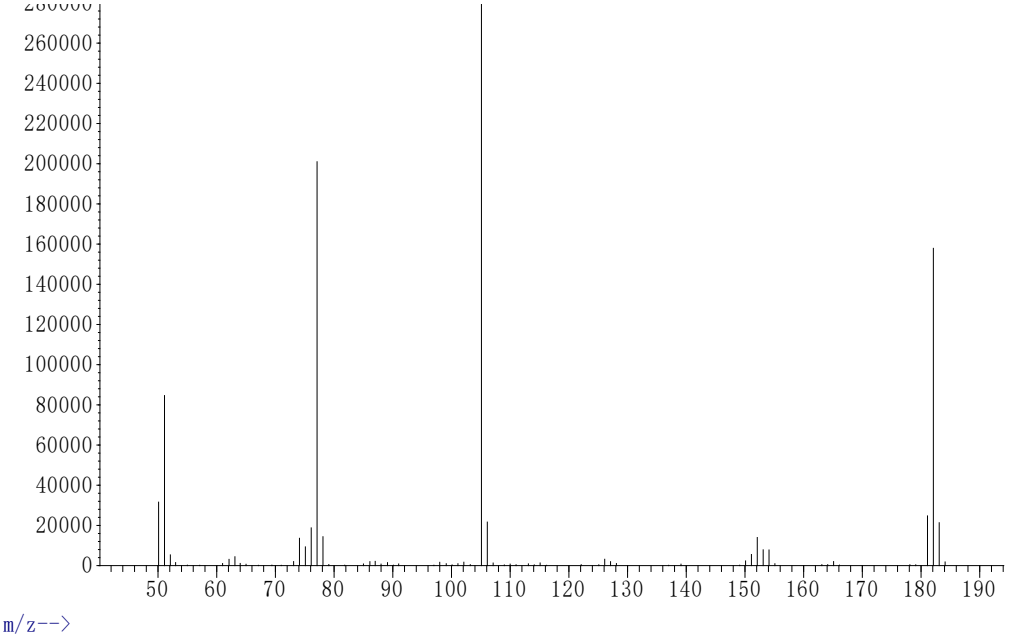
Run	Time /min	Start scanning	Peak scanning	Stop scanning	Peak type	Hight	Correction area	Correction maximum%	Total%
1	6.939	478	484	510	M	742092	33350179	24.94	**19.964**
2	7.651	567	571	650	M	1691586	133697340	100.00	**80.036**

MS Spectra

T = 6.939 min, m/z =180,  (**7b**)

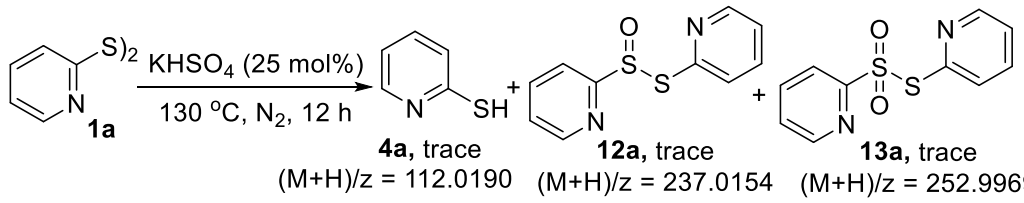


T = 7.651 min, m/z = 182,  (**8b**)

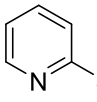


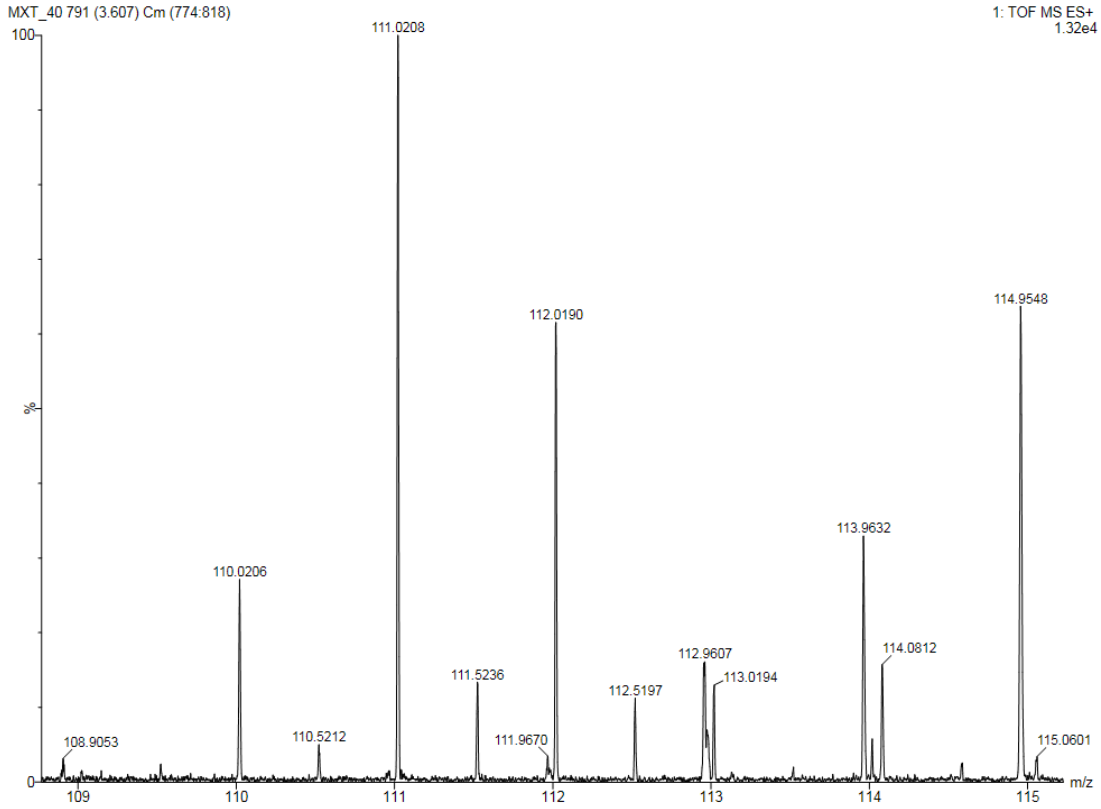
Results and Discussion: The reaction of **7b** with H_2O_2 could effectively afford **8b** in 70% isolated yield, suggesting that H_2O_2 should be the most possible active oxidizing species generated through the oxidation of H_2O.

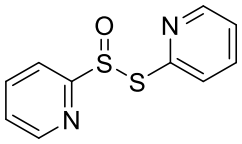
3.3 ESI-HRMS analysis of the key intermediates (eq. 7 in the main text)

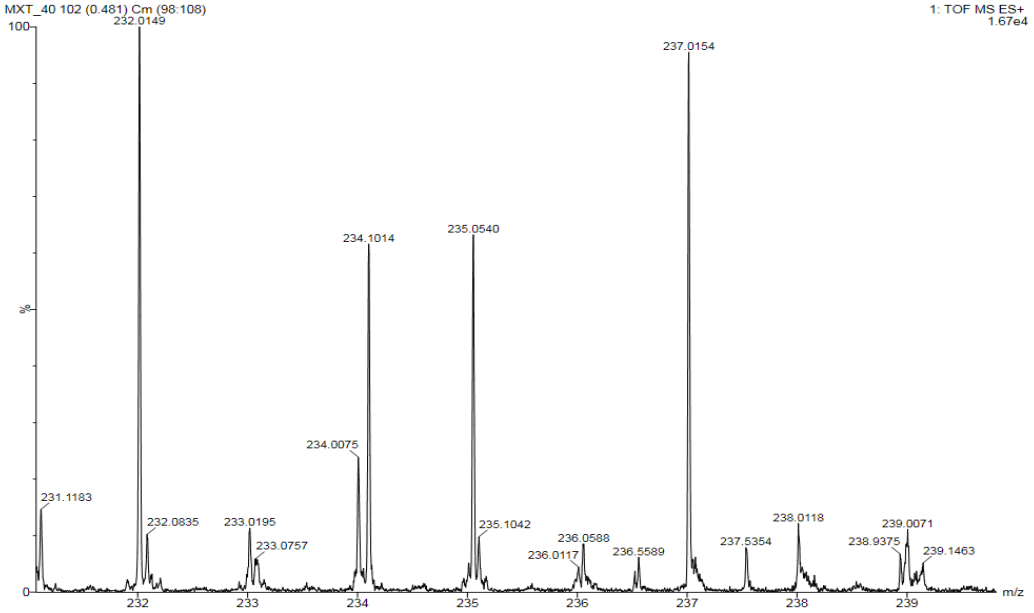


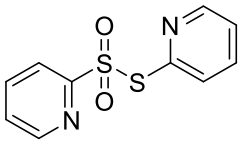
Detailed Procedure: The mixture of di(pyridin-2-yl)disulfide **1a** (82.5 mg, 0.375 mmol) and $KHSO_4$ (17.0 mg, 0.125 mmol, 25 mol%) was directly sealed in a Schlenk tube (10 mL) under nitrogen, and stirred at 130 °C for 2 h. The reaction mixture was then analyzed by ESI-HRMS.

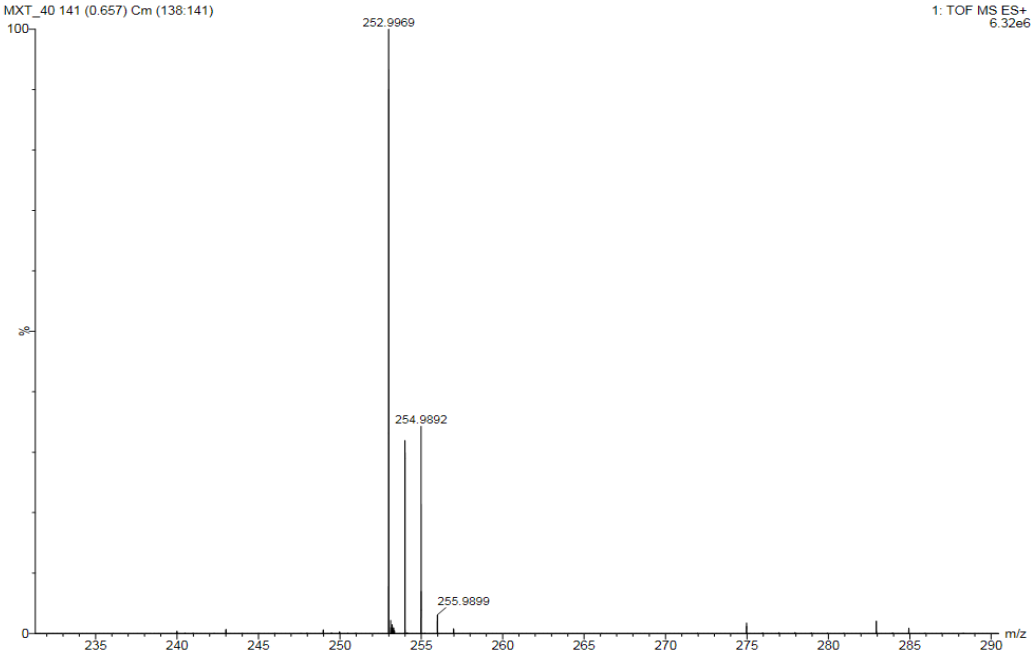
HRMS Spectra of  **(4a)**



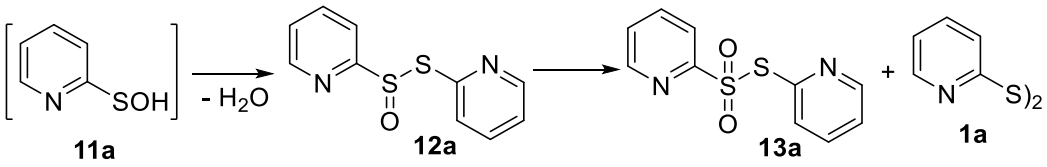
HRMS Spectra of  **(12a)**



HRMS Spectra of  **(13a)**



Results and Discussion: HRMS analysis of the $KHSO_4$-catalyzed blank reaction of **1a** showed the generation of trace yields of 2-PySH (**4a**), thiosulfinate **12a**, and thiolsulfonate **13a**. Clearly, the production of **4a** confirmed again the heterolytic cleavage of S-S bond by acid catalysis; whereas, as shown by the scheme below, **12a** and **13a** are in effect the characteristic products of the stepwise disproportionation reactions of sulfenic acids 2-PySOH (**11a**), implying that **11a** were most possibly generated in the process by the reaction of 2-PyS^+ (**10a**) with water.



11a **12a** **13a** **1a**

4. Density Functional Theory (DFT) Calculation Studies

Summary table for the Key Intermediates

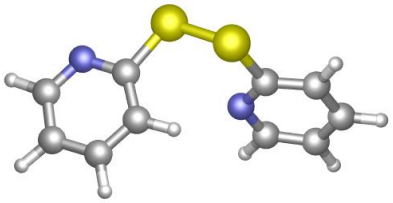
Run	Structure	E_0	H_{298}	G_{298}	TCGFE
1	**1a**	-1291.613503	-1291.600528	-1291.654395	0.119658
2	**1a-H$^+$**	-1291.982235	-1291.969190	-1292.022745	0.134138
3	**1a-H$^+$'**	-1291.933610	-1291.920357	-1291.975057	0.129341
4	**TS1**	-1291.939669	-1291.926599	-1291.982043	0.130527
5	**TS1'**	-1291.892567	-1291.880150	-1291.931988	0.128683
6	**14a**	-1291.947738	-1291.935146	-1291.987157	0.133704
7	**14a'**	-1291.896766	-1291.883289	-1291.939226	0.125765
8	**15a**	-1291.901210	-1291.888228	-1291.942367	0.130942
9	**15a'**	-1291.882636	-1291.869193	-1291.924361	0.125923
10	**H_2O**	-76.387796	-76.384017	-76.405463	0.003499
11	**4a'**	-646.395183	-646.388675	-646.425041	0.062249
12	**4a**	-646.393999	-646.387114	-646.424095	0.057924
13	**10a**	-645.446506	-645.439805	-645.476846	0.048146
14	**16a**	-2013.554089	-2013.532515	-2013.607003	0.214234
15	**16a'**	-2013.525485	-2013.502852	-2013.583622	0.206703
16	**17a**	-2013.601334	-2013.579662	-2013.657573	0.213205
17	**17a'**	-2013.543597	-2013.521720	-2013.598451	0.211095
18	**11a**	-721.582802	-721.574833	-721.614898	0.061486
19	**18a**	-1443.186721	-1443.170389	-1443.232328	0.143947
20	**19a**	-1443.138418	-1443.121379	-1443.185181	0.143037

E_0: Sum of electronic and zero-point Energies

H_{298}: Sum of electronic and thermal Enthalpies

G_{298}: Sum of electronic and thermal Free Energies

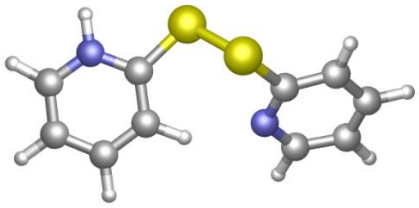
TCGFE: Thermal correction to Gibbs Free Energy



1a

Standard orientation:

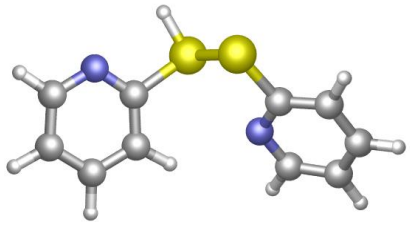
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.975385	0.467485	-0.541946
2	6	0	3.828909	1.459786	0.425665
3	6	0	2.621111	1.522867	1.124707
4	6	0	1.614528	0.605062	0.838998
5	6	0	1.882148	-0.356851	-0.140938
6	7	0	3.024486	-0.432718	-0.821761
7	1	0	2.459471	2.286482	1.881050
8	1	0	4.894243	0.381088	-1.118743
9	1	0	4.633721	2.161266	0.621551
10	1	0	0.657878	0.637009	1.344090
11	16	0	0.733857	-1.632276	-0.694514
12	16	0	-0.809156	-1.661187	0.690276
13	6	0	-1.926044	-0.340618	0.163147
14	6	0	-3.272547	-0.445732	0.542095
15	6	0	-4.127340	0.595863	0.194261
16	1	0	-3.634233	-1.318596	1.076862
17	6	0	-2.266185	1.674987	-0.855025
18	6	0	-3.619729	1.682184	-0.522823
19	1	0	-5.178518	0.553091	0.466192
20	1	0	-1.825654	2.496441	-1.416615
21	1	0	-4.255219	2.510155	-0.820434
22	7	0	-1.425671	0.689615	-0.511809



1a-H$^+$

Standard orientation:

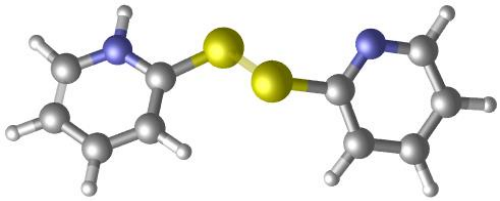
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.205267	0.168771	-0.276127
2	6	0	3.986265	1.407889	0.285120
3	6	0	2.668957	1.781384	0.598693
4	6	0	1.605038	0.922711	0.341318
5	6	0	1.860491	-0.330678	-0.220332
6	7	0	3.151955	-0.658636	-0.498397
7	1	0	2.473750	2.758744	1.029442
8	1	0	5.181790	-0.211479	-0.551197
9	1	0	4.824445	2.068802	0.471617
10	1	0	0.568982	1.202795	0.518367
11	16	0	0.645897	-1.544321	-0.676385
12	16	0	-0.747813	-1.460619	0.883867
13	6	0	-1.991113	-0.296628	0.276280
14	6	0	-3.317846	-0.728832	0.219074
15	6	0	-4.284893	0.205824	-0.159394
16	1	0	-3.581511	-1.754688	0.452117
17	6	0	-2.521960	1.813980	-0.415055
18	6	0	-3.881589	1.498258	-0.487524
19	1	0	-5.330599	-0.081347	-0.212435
20	1	0	-2.167483	2.809051	-0.671819
21	1	0	-4.598909	2.250502	-0.798257
22	7	0	-1.587563	0.939417	-0.023143
23	1	0	3.337748	-1.584910	-0.879075



1a-H^{+},

Standard orientation:

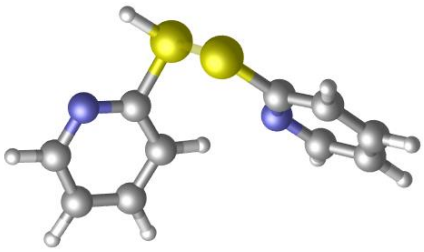
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.412326	1.639305	-0.617475
2	6	0	-3.731357	1.590317	-0.170660
3	6	0	-4.165368	0.451461	0.510260
4	6	0	-3.276450	-0.603901	0.719377
5	6	0	-1.976103	-0.431138	0.245359
6	7	0	-1.535277	0.647066	-0.395400
7	1	0	-5.189690	0.373002	0.861145
8	1	0	-2.033862	2.496935	-1.166618
9	1	0	-4.401409	2.421826	-0.359652
10	1	0	-3.588324	-1.517165	1.215219
11	16	0	-0.755136	-1.732692	0.535663
12	16	0	0.530203	-1.112741	-1.036049
13	6	0	1.895123	-0.134915	-0.318735
14	6	0	1.737558	1.233361	-0.120272
15	6	0	2.855661	1.904407	0.382508
16	1	0	0.800061	1.732187	-0.332855
17	6	0	4.044573	-0.191809	0.393196
18	6	0	4.022735	1.185428	0.641409
19	1	0	2.810696	2.973352	0.565593
20	1	0	4.933531	-0.786857	0.580793
21	1	0	4.906632	1.678230	1.032385
22	7	0	2.981779	-0.854024	-0.081226
23	1	0	1.271520	-2.250978	-1.043258



TS1

Standard orientation:

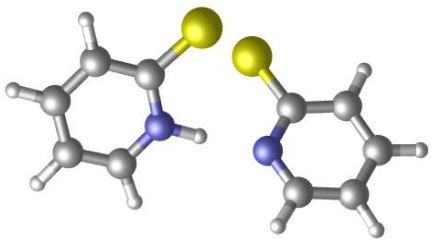
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.655628	0.559281	0.184248
2	6	0	4.806178	-0.798932	0.028045
3	6	0	3.648738	-1.597449	-0.031365
4	6	0	2.389726	-1.028775	0.081414
5	6	0	2.251928	0.362719	0.243927
6	7	0	3.409609	1.093682	0.266636
7	1	0	3.741186	-2.672484	-0.152319
8	1	0	5.480693	1.259492	0.239154
9	1	0	5.797993	-1.227857	-0.048264
10	1	0	1.491897	-1.633425	0.048831
11	16	0	0.763092	1.231622	0.452869
12	16	0	-0.823309	-0.267480	-1.237279
13	6	0	-2.354048	-0.167514	-0.419194
14	6	0	-2.796460	-1.257946	0.365442
15	6	0	-4.077520	-1.206049	0.912281
16	1	0	-2.149743	-2.114584	0.519033
17	6	0	-4.301870	0.985043	-0.083943
18	6	0	-4.844391	-0.066383	0.686491
19	1	0	-4.461026	-2.030497	1.505080
20	1	0	-4.880003	1.889292	-0.259380
21	1	0	-5.844779	0.027161	1.097423
22	7	0	-3.095368	0.944686	-0.631264
23	1	0	3.320114	2.104065	0.349325



TS1'

Standard orientation:

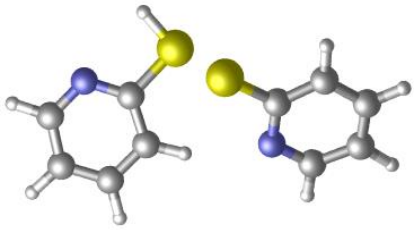
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.182201	1.564216	0.723135
2	6	0	3.499601	1.743843	0.238646
3	6	0	4.067235	0.747214	-0.551763
4	6	0	3.316845	-0.394049	-0.819538
5	6	0	1.998264	-0.484869	-0.289587
6	7	0	1.441052	0.497581	0.468126
7	1	0	5.075647	0.847098	-0.940437
8	1	0	1.726203	2.329152	1.347927
9	1	0	4.048889	2.644515	0.492928
10	1	0	3.715879	-1.203122	-1.421728
11	16	0	1.068324	-1.891501	-0.654215
12	16	0	-0.958506	-1.347069	1.353760
13	6	0	-1.985635	-0.226001	0.436686
14	6	0	-1.789379	1.154198	0.591885
15	6	0	-2.640499	1.997663	-0.119396
16	1	0	-1.011361	1.539242	1.240668
17	6	0	-3.713376	0.037024	-1.021033
18	6	0	-3.619723	1.434862	-0.938786
19	1	0	-2.541797	3.075149	-0.032150
20	1	0	-4.461194	-0.436180	-1.651805
21	1	0	-4.300848	2.058347	-1.508290
22	7	0	-2.908333	-0.788079	-0.349409
23	1	0	-1.630736	-2.448198	0.947661



14a

Standard orientation:

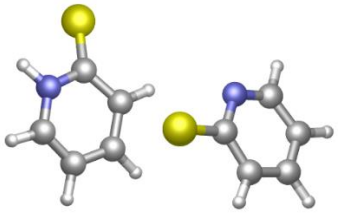
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.147301	1.731234	0.515572
2	6	0	-3.530177	1.688077	0.520971
3	6	0	-4.160214	0.525380	0.059056
4	6	0	-3.400411	-0.557813	-0.373200
5	6	0	-1.997802	-0.471935	-0.388677
6	7	0	-1.430741	0.688523	0.050213
7	1	0	-5.243538	0.453708	0.064227
8	1	0	-1.573132	2.578428	0.873244
9	1	0	-4.096989	2.535164	0.888618
10	1	0	-3.870664	-1.480497	-0.692832
11	16	0	-1.007548	-1.764612	-1.007294
12	16	0	0.980891	-1.551194	1.175674
13	6	0	1.986361	-0.363088	0.396829
14	6	0	3.353409	-0.638833	0.194650
15	6	0	4.178994	0.374083	-0.299446
16	1	0	3.744459	-1.621724	0.432616
17	6	0	2.220286	1.765256	-0.462154
18	6	0	3.606501	1.595143	-0.637266
19	1	0	5.240589	0.197283	-0.440856
20	1	0	1.740192	2.695477	-0.755297
21	1	0	4.200776	2.404742	-1.047473
22	7	0	1.431895	0.830914	0.059519
23	1	0	-0.381134	0.769235	0.057531



14a′

Standard orientation:

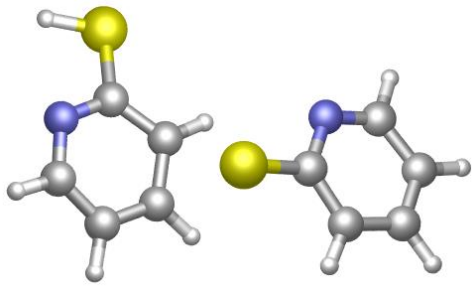
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.468810	1.624307	0.572288
2	6	0	3.871584	1.551992	0.395594
3	6	0	4.418974	0.411681	-0.185309
4	6	0	3.557276	-0.612309	-0.571285
5	6	0	2.158394	-0.437612	-0.383870
6	7	0	1.626892	0.674970	0.195543
7	1	0	5.490622	0.313671	-0.326557
8	1	0	2.028777	2.498357	1.047237
9	1	0	4.498215	2.374395	0.725161
10	1	0	3.931248	-1.527252	-1.018054
11	16	0	1.088027	-1.663492	-0.950268
12	16	0	-0.914759	-1.093245	1.366709
13	6	0	-2.133840	-0.183210	0.466389
14	6	0	-1.852355	1.143323	0.095315
15	6	0	-2.856660	1.839409	-0.572453
16	1	0	-0.882334	1.580949	0.303489
17	6	0	-4.224140	-0.144863	-0.431443
18	6	0	-4.064586	1.192172	-0.837395
19	1	0	-2.697759	2.866993	-0.883767
20	1	0	-5.147572	-0.681004	-0.633663
21	1	0	-4.870775	1.699196	-1.357120
22	7	0	-3.276842	-0.830247	0.206330
23	1	0	-1.633824	-2.239916	1.380114



15a

Standard orientation:

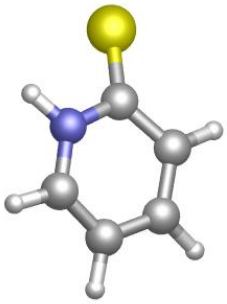
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.180883	-1.673726	-0.118635
2	6	0	-2.028540	-2.073171	-0.762959
3	6	0	-0.999089	-1.134559	-0.931143
4	6	0	-1.152595	0.192461	-0.444990
5	6	0	-2.469235	0.647773	-0.011899
6	7	0	-3.365644	-0.386250	0.254319
7	1	0	-0.111452	-1.389465	-1.499905
8	1	0	-4.003511	-2.349681	0.087956
9	1	0	-1.922738	-3.096061	-1.100718
10	1	0	-0.405566	0.955768	-0.630948
11	16	0	-3.004239	2.234484	-0.032276
12	16	0	0.623890	-0.993086	1.159140
13	6	0	2.007782	-0.255752	0.416939
14	6	0	3.060915	-1.085032	-0.042280
15	6	0	4.238336	-0.479320	-0.479995
16	1	0	2.953724	-2.164250	-0.020714
17	6	0	3.162244	1.652422	-0.106394
18	6	0	4.294792	0.911081	-0.512542
19	1	0	5.081559	-1.081343	-0.803702
20	1	0	3.169496	2.738320	-0.164620
21	1	0	5.182504	1.429998	-0.859772
22	7	0	2.053392	1.097872	0.362391
23	1	0	-4.275041	-0.100066	0.609006



15a'

Standard orientation:

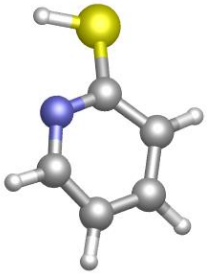
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.144753	1.709947	-0.009598
2	6	0	2.011106	2.140659	-0.701622
3	6	0	1.006352	1.209853	-0.941283
4	6	0	1.170773	-0.137677	-0.477959
5	6	0	2.503214	-0.500984	-0.020313
6	7	0	3.407807	0.420311	0.270307
7	1	0	0.117903	1.470815	-1.506016
8	1	0	3.913898	2.416485	0.292019
9	1	0	1.910804	3.173329	-1.014271
10	1	0	0.446147	-0.909559	-0.715979
11	16	0	3.052431	-2.195094	-0.070285
12	16	0	-0.638851	0.950982	1.144887
13	6	0	-2.013224	0.221612	0.400805
14	6	0	-3.051565	1.064479	-0.075721
15	6	0	-4.246852	0.475864	-0.488958
16	1	0	-2.917968	2.140976	-0.082372
17	6	0	-3.208715	-1.672902	-0.072740
18	6	0	-4.330874	-0.912700	-0.487381
19	1	0	-5.079482	1.087761	-0.821069
20	1	0	-3.243082	-2.759237	-0.109115
21	1	0	-5.231676	-1.421183	-0.816383
22	7	0	-2.086764	-1.134563	0.374885
23	1	0	4.309053	-1.882745	0.311826



4a’

Standard orientation:

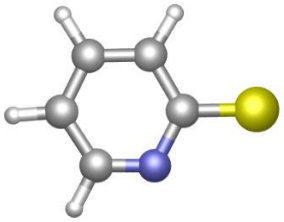
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.488502	-1.189382	-0.000139
2	6	0	2.243288	-0.050854	-0.000084
3	6	0	1.560446	1.197792	-0.000109
4	6	0	0.190030	1.252334	-0.000067
5	6	0	-0.615379	0.063651	0.000802
6	7	0	0.127782	-1.111415	0.000264
7	1	0	2.135420	2.119956	0.000366
8	1	0	1.906315	-2.189885	-0.000904
9	1	0	3.324783	-0.110063	-0.000533
10	1	0	-0.336792	2.199116	0.000205
11	16	0	-2.293744	0.005105	-0.000252
12	1	0	-0.425619	-1.962156	0.000629



4a

Standard orientation:

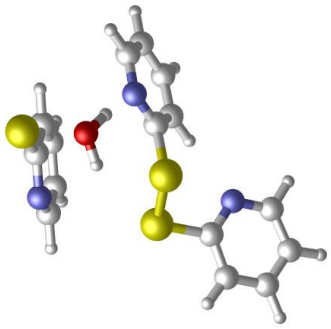
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.451073	-1.222134	-0.000034
2	6	0	2.257415	-0.086484	-0.000033
3	6	0	1.629801	1.162269	0.000050
4	6	0	0.241355	1.223772	0.000034
5	6	0	-0.472475	0.014341	0.000026
6	7	0	0.110781	-1.186358	0.000004
7	1	0	2.215774	2.077440	0.000073
8	1	0	1.893213	-2.216755	-0.000056
9	1	0	3.338849	-0.177430	-0.000051
10	1	0	-0.280213	2.175950	-0.000022
11	16	0	-2.260837	0.072607	-0.000063
12	1	0	-2.412711	-1.267003	0.000784



10a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	2.228002	0.005512	-0.000310
2	6	0	0.566264	-0.023513	0.000371
3	6	0	-0.169490	1.233400	0.000480
4	6	0	-1.556128	1.208929	-0.000092
5	1	0	0.388404	2.165094	0.000815
6	6	0	-1.378469	-1.250343	-0.000098
7	6	0	-2.171082	-0.043236	-0.000440
8	1	0	-2.139225	2.124250	-0.000158
9	1	0	-1.878395	-2.216564	0.000317
10	1	0	-3.254981	-0.129003	-0.000944
11	7	0	-0.072915	-1.254770	0.000514

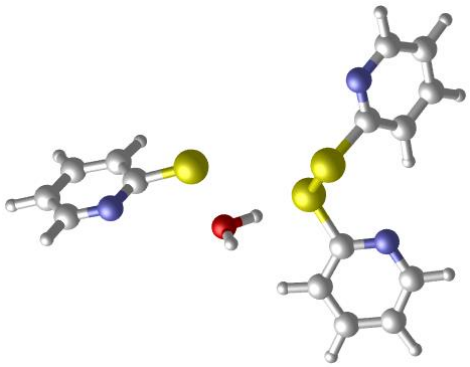


16a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.099244	2.767219	-0.393306
2	6	0	1.526218	3.483686	0.651678
3	6	0	0.265666	3.091215	1.113648
4	6	0	-0.383083	2.012631	0.516995
5	6	0	0.284959	1.343409	-0.512921
6	7	0	1.499008	1.701297	-0.951920
7	1	0	-0.220117	3.638885	1.916144
8	1	0	3.072032	3.032944	-0.797765
9	1	0	2.048232	4.331558	1.082202
10	1	0	-1.387475	1.708072	0.795083
11	16	0	-0.434697	-0.027261	-1.439985
12	16	0	-1.422022	-1.208321	-0.029032
13	6	0	-3.131642	-0.618548	-0.083117
14	6	0	-4.140950	-1.555279	-0.320863
15	6	0	-5.462563	-1.105974	-0.280838
16	1	0	-3.900727	-2.589760	-0.541207
17	6	0	-4.619934	1.094608	0.168130
18	6	0	-5.709154	0.243735	-0.037189
19	1	0	-6.280704	-1.798052	-0.456341
20	1	0	-4.769436	2.155626	0.352579
21	1	0	-6.720277	0.636276	-0.010643
22	7	0	-3.349803	0.672969	0.163278
23	6	0	1.349395	-2.395720	1.461986
24	6	0	1.244286	-1.426246	2.484981
25	6	0	2.039688	-0.286686	2.429167
26	6	0	2.907827	-0.141828	1.347379
27	6	0	2.947993	-1.170255	0.381155
28	7	0	2.176014	-2.281935	0.433786

29	1	0	1.978525	0.478768	3.195714
30	1	0	0.730518	-3.288614	1.488198
31	1	0	0.542830	-1.580400	3.298613
32	1	0	3.534436	0.735358	1.237499
33	16	0	4.063511	-1.053462	-0.943038
34	8	0	2.761534	-0.371501	-2.442967
35	1	0	2.372466	0.484086	-2.069152
36	1	0	2.014518	-1.010164	-2.431625

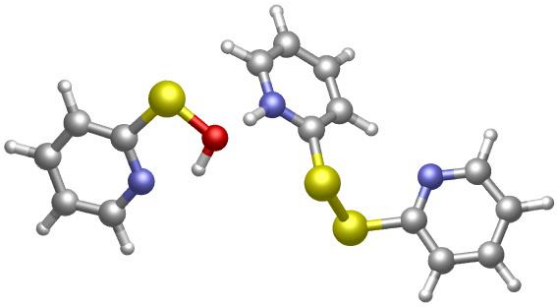


16a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.703524	3.158793	-0.144628
2	6	0	3.078597	4.408477	-0.127987
3	6	0	1.705505	4.464278	0.105458
4	6	0	1.003999	3.273238	0.305063
5	6	0	1.739252	2.086482	0.278075
6	7	0	3.047240	2.011451	0.067831
7	1	0	1.182448	5.415748	0.120847
8	1	0	4.771213	3.069772	-0.327405
9	1	0	3.657678	5.310238	-0.296541
10	1	0	-0.068781	3.271991	0.472793
11	16	0	0.887210	0.518619	0.628515
12	16	0	1.371988	-0.762781	-0.968588
13	6	0	2.667351	-1.831702	-0.286295
14	6	0	3.777733	-1.320084	0.390469
15	6	0	4.725525	-2.244184	0.828480
16	1	0	3.892192	-0.252519	0.544911
17	6	0	3.407105	-3.980551	-0.175982
18	6	0	4.541622	-3.598036	0.540865
19	1	0	5.604607	-1.907403	1.370208
20	1	0	3.232495	-5.022017	-0.434423
21	1	0	5.262876	-4.343526	0.859586
22	7	0	2.465246	-3.112628	-0.572519
23	6	0	-6.271052	0.135287	-0.736563
24	6	0	-6.790273	-0.128689	0.550944
25	6	0	-5.946955	-0.630327	1.537243
26	6	0	-4.608066	-0.848883	1.210261
27	6	0	-4.193722	-0.581946	-0.112923

28	7	0	-5.010267	-0.091032	-1.074799
29	1	0	-6.314906	-0.838664	2.536788
30	1	0	-6.915400	0.536596	-1.515030
31	1	0	-7.838835	0.063469	0.756286
32	1	0	-3.898129	-1.222741	1.939983
33	16	0	-2.572038	-0.976831	-0.581794
34	8	0	-1.740950	0.948412	-0.468957
35	1	0	-1.627063	1.206044	-1.406240
36	1	0	-0.763765	0.834150	-0.038701

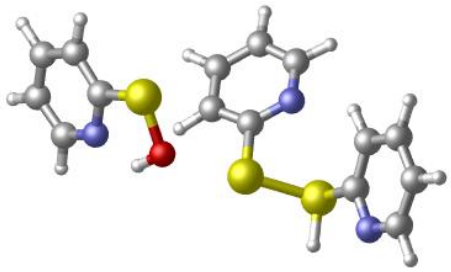


17a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.947785	2.676706	-0.276124
2	6	0	-0.119630	3.521039	-0.987626
3	6	0	1.191345	3.100439	-1.256476
4	6	0	1.644156	1.861671	-0.813059
5	6	0	0.766591	1.033307	-0.109195
6	7	0	-0.494804	1.468168	0.128649
7	1	0	1.868377	3.753012	-1.799419
8	1	0	-1.973645	2.904426	-0.011046
9	1	0	-0.485731	4.485847	-1.318132
10	1	0	2.669526	1.532794	-0.952527
11	16	0	1.155451	-0.563278	0.581297
12	16	0	2.441651	-1.419615	-0.825506
13	6	0	4.089796	-0.987804	-0.217009
14	6	0	5.002414	-2.024316	-0.006216
15	6	0	6.298042	-1.675334	0.380920
16	1	0	4.707369	-3.060718	-0.129334
17	6	0	5.608900	0.622135	0.344990
18	6	0	6.607823	-0.329373	0.565887
19	1	0	7.043319	-2.446239	0.552040
20	1	0	5.808305	1.681532	0.486430
21	1	0	7.598494	-0.016808	0.878877
22	7	0	4.371921	0.305625	-0.056814
23	6	0	-4.383204	-2.215117	-0.816441
24	6	0	-5.665004	-2.052329	-1.329752
25	6	0	-6.407958	-0.934566	-0.930885
26	6	0	-5.853005	-0.020416	-0.040343
27	6	0	-4.557019	-0.281796	0.412431
28	7	0	-3.838051	-1.339428	0.043867

29	1	0	-7.412744	-0.778017	-1.311694
30	1	0	-3.764410	-3.065254	-1.088942
31	1	0	-6.073044	-2.781249	-2.021168
32	1	0	-6.402174	0.855225	0.291776
33	16	0	-3.725260	0.771032	1.608091
34	8	0	-2.228958	-0.052195	1.567247
35	1	0	-1.158778	0.840964	0.649664
36	1	0	-2.468919	-0.904187	1.076864

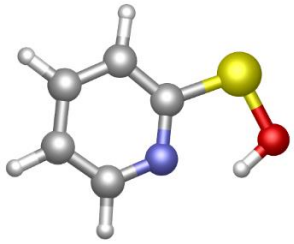


17a'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.572267	3.054897	0.440840
2	6	0	-0.759357	3.448464	0.306608
3	6	0	-1.665663	2.544366	-0.246054
4	6	0	-1.219508	1.283566	-0.643141
5	6	0	0.125736	0.984196	-0.426365
6	7	0	1.008564	1.834717	0.097940
7	1	0	-2.707133	2.817619	-0.386810
8	1	0	1.320849	3.733348	0.841238
9	1	0	-1.068399	4.441228	0.615694
10	1	0	-1.888812	0.567842	-1.102725
11	16	0	0.768072	-0.655225	-0.853129
12	16	0	2.657054	0.171574	-1.591182
13	6	0	3.934990	-0.244441	-0.355965
14	6	0	3.962282	0.424836	0.863810
15	6	0	4.999616	0.068805	1.728494
16	1	0	3.208056	1.161384	1.115857
17	6	0	5.776740	-1.493234	0.070523
18	6	0	5.921026	-0.899675	1.327495
19	1	0	5.083772	0.544582	2.700635
20	1	0	6.469348	-2.253755	-0.278533
21	1	0	6.737402	-1.197673	1.976871
22	7	0	4.783121	-1.172718	-0.770308
23	6	0	-4.825704	-0.922434	-1.323118
24	6	0	-5.957238	-0.385212	-0.721066
25	6	0	-5.904429	-0.079240	0.645120
26	6	0	-4.735440	-0.317341	1.359869
27	6	0	-3.656190	-0.865419	0.657560
28	7	0	-3.690545	-1.159163	-0.643029
29	1	0	-6.770168	0.341966	1.147496

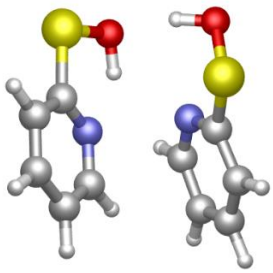
30	1	0	-4.810876	-1.179575	-2.378517
31	1	0	-6.856277	-0.212794	-1.302327
32	1	0	-4.661800	-0.092997	2.419589
33	16	0	-2.109217	-1.269290	1.459214
34	8	0	-1.277728	-1.758666	0.063884
35	1	0	-2.010211	-1.822377	-0.622616
36	1	0	2.998793	-0.865081	-2.395244



11a

Standard orientation:

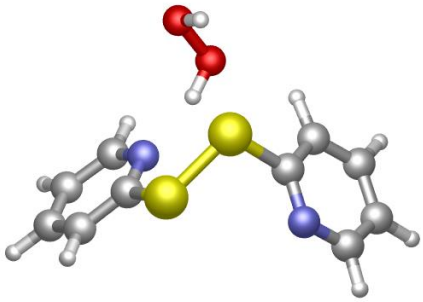
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.478173	1.350483	-0.000240
2	6	0	-2.509498	0.418778	0.000002
3	6	0	-2.171037	-0.941941	0.000120
4	6	0	-0.835106	-1.315983	0.000165
5	6	0	0.128308	-0.293126	0.000128
6	7	0	-0.181789	1.006097	-0.000084
7	1	0	-2.947615	-1.701857	0.000280
8	1	0	-1.684583	2.418235	-0.000204
9	1	0	-3.544381	0.743923	0.000063
10	1	0	-0.538285	-2.360731	0.000279
11	16	0	1.866718	-0.647274	-0.000291
12	8	0	2.459821	0.927833	0.000522
13	1	0	1.634364	1.482196	-0.000393



18a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.357319	0.359228	1.653019
2	6	0	3.041340	1.486865	1.202530
3	6	0	3.134274	1.688815	-0.179114
4	6	0	2.552156	0.765579	-1.038734
5	6	0	1.873824	-0.330137	-0.476671
6	7	0	1.769717	-0.529586	0.840792
7	1	0	3.668160	2.547091	-0.578726
8	1	0	2.260589	0.158907	2.718424
9	1	0	3.491174	2.177609	1.908521
10	1	0	2.629663	0.872368	-2.117025
11	16	0	1.030306	-1.458660	-1.569218
12	8	0	0.869971	-2.830640	-0.642681
13	1	0	0.164782	-2.640175	0.025617
14	6	0	-0.725898	1.962605	0.262861
15	6	0	-1.594968	2.771938	-0.462137
16	6	0	-2.823928	2.232017	-0.862466
17	6	0	-3.135398	0.916773	-0.539036
18	6	0	-2.185530	0.192605	0.195986
19	7	0	-1.022955	0.700146	0.597430
20	1	0	-3.527197	2.830187	-1.435320
21	1	0	0.246282	2.319934	0.593407
22	1	0	-1.319485	3.791498	-0.710545
23	1	0	-4.068444	0.459880	-0.855000
24	16	0	-2.469772	-1.494160	0.692417
25	8	0	-0.905796	-1.884605	1.213250
26	1	0	-0.413943	-1.021872	1.309940

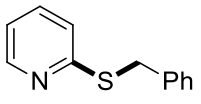


19a

Standard orientation:

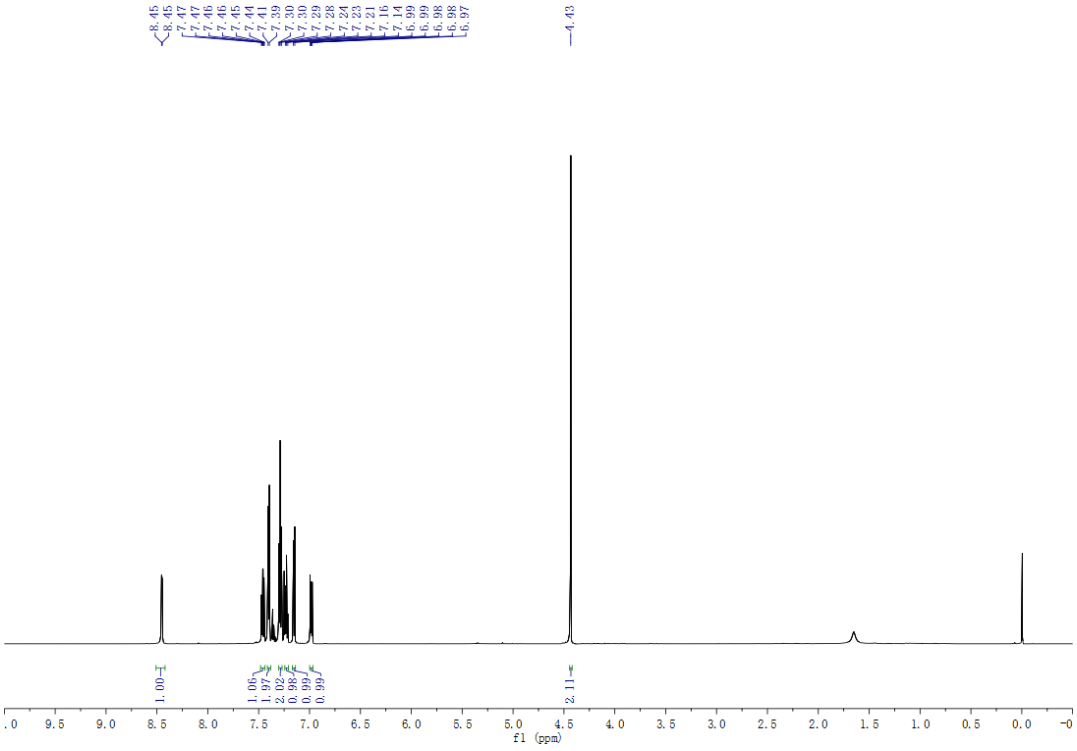
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.351094	-1.591492	-0.811643
2	6	0	3.864096	-0.544418	-1.581075
3	6	0	3.366997	0.739755	-1.363769
4	6	0	2.382810	0.932064	-0.393399
5	6	0	1.966878	-0.189842	0.332951
6	7	0	2.428856	-1.423362	0.142101
7	1	0	3.721706	1.580987	-1.953000
8	1	0	3.701338	-2.611532	-0.958347
9	1	0	4.623413	-0.737967	-2.332495
10	1	0	1.920968	1.900310	-0.230023
11	16	0	0.771568	0.070924	1.673523
12	8	0	-0.844912	3.226663	1.073870
13	1	0	-0.189880	2.941528	1.737581
14	6	0	-2.543846	0.783542	-1.277993
15	6	0	-3.652418	0.026649	-1.636273
16	6	0	-3.817022	-1.223507	-1.031224
17	6	0	-2.880797	-1.658677	-0.101657
18	6	0	-1.794314	-0.817242	0.189863
19	7	0	-1.625688	0.367965	-0.388799
20	1	0	-4.669477	-1.850414	-1.277767
21	1	0	-2.364372	1.769363	-1.699964
22	1	0	-4.365451	0.404168	-2.361474
23	1	0	-2.983265	-2.620904	0.391080
24	16	0	-0.615180	-1.442688	1.404068
25	8	0	-0.208874	2.770792	-0.149289
26	1	0	-0.549936	1.839827	-0.181486

5. Copies of the ^{1}H, ^{13}C NMR and IR Spectra of the Products

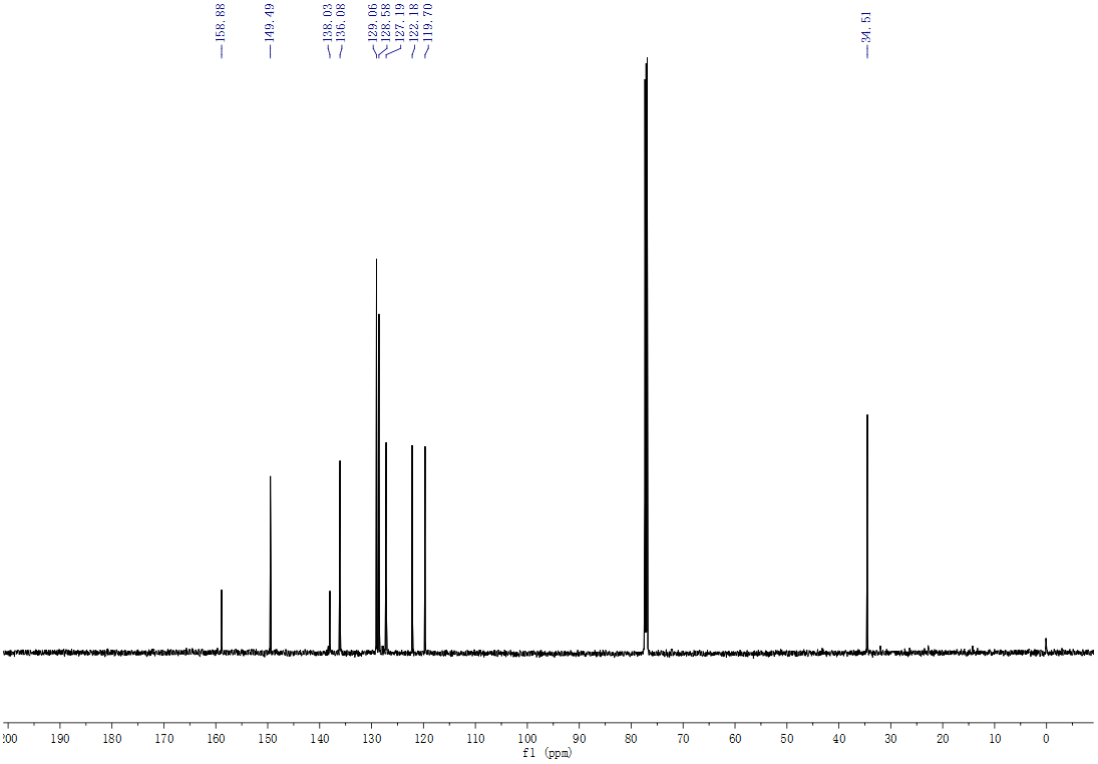


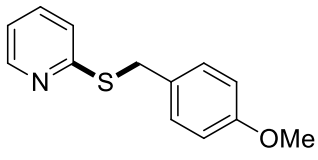
3aa

^{1}H NMR ($CDCl_3$, 600 M Hz)



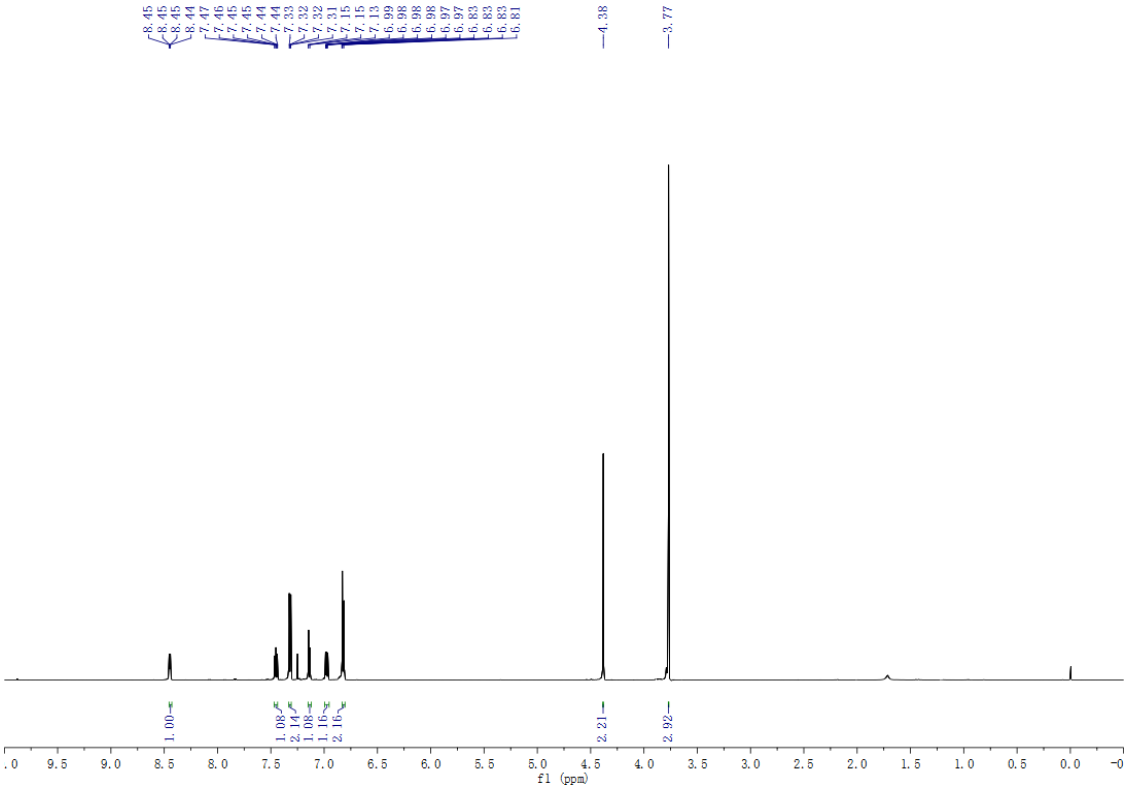
^{13}C NMR ($CDCl_3$, 150 M Hz)



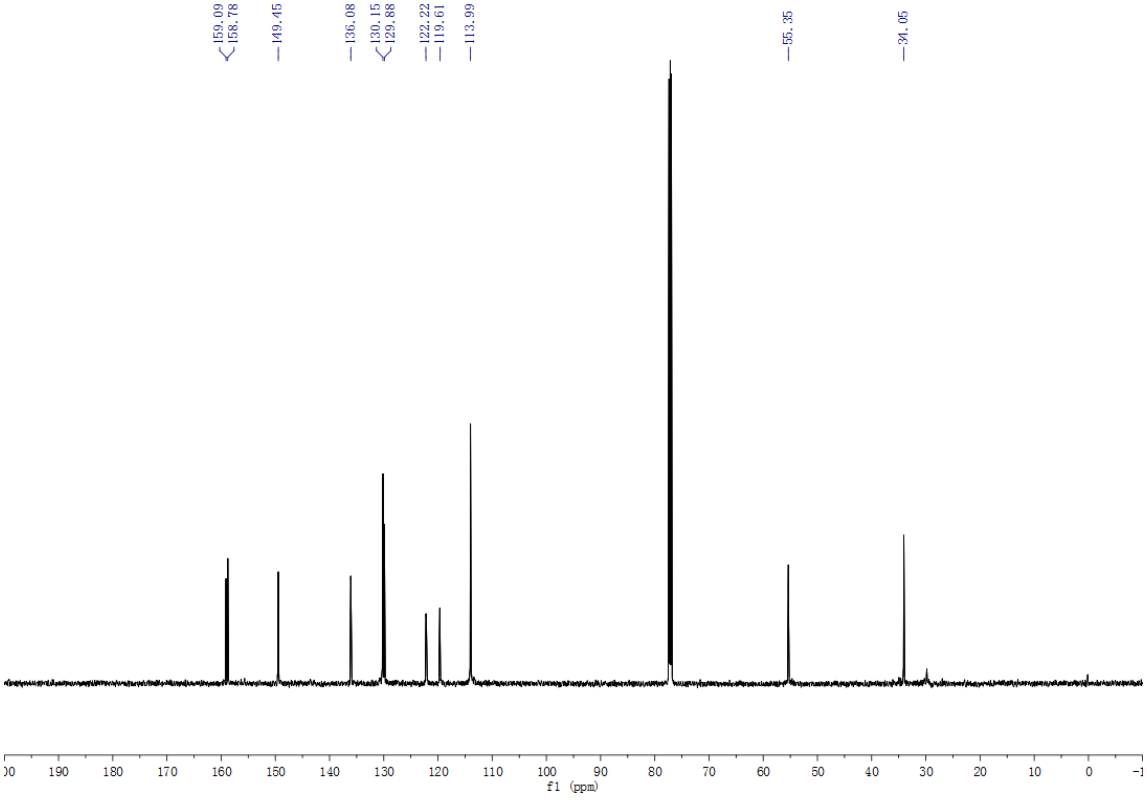


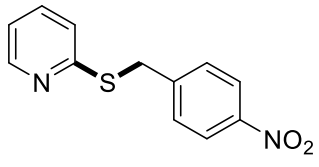
3ab

^{1}H NMR ($CDCl_3$, 600 M Hz)



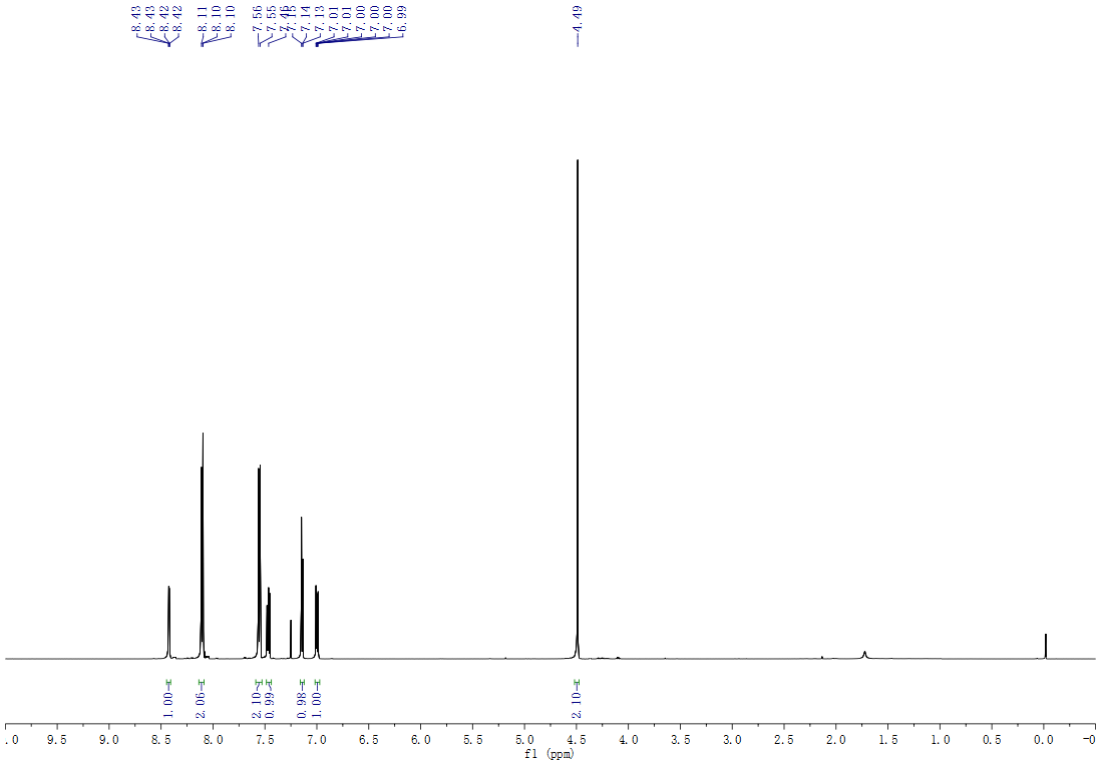
^{13}C NMR ($CDCl_3$, 150 M Hz)



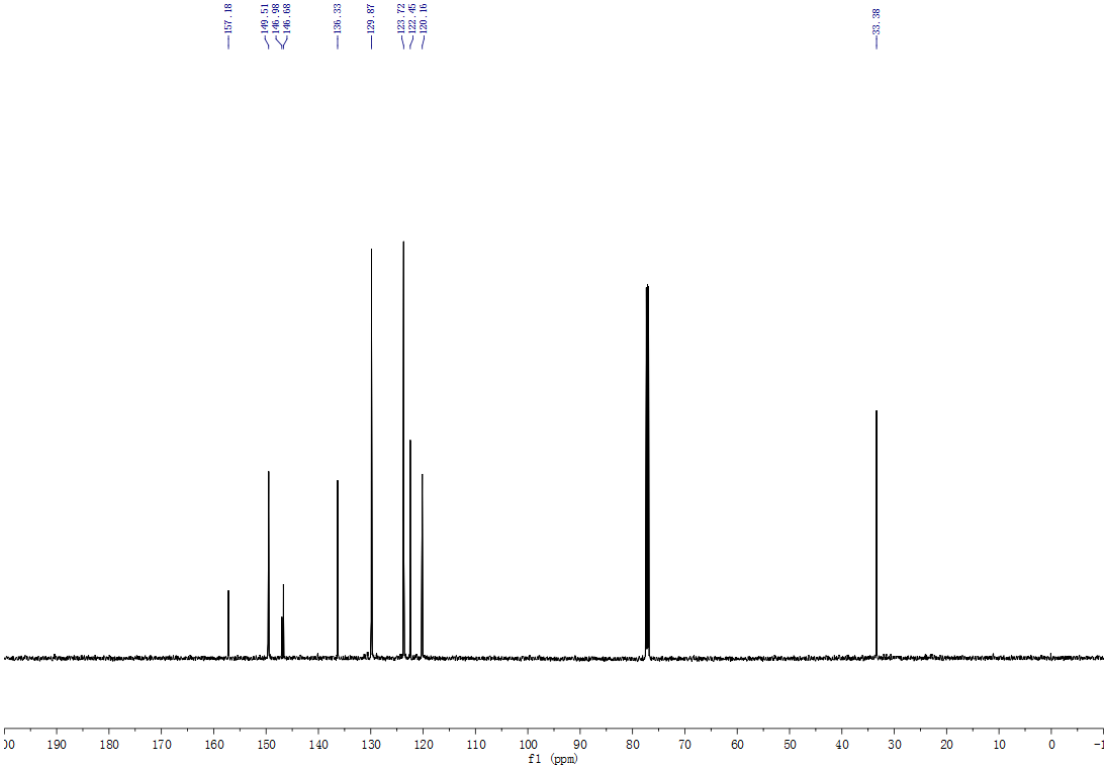


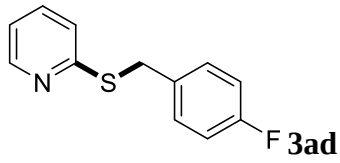
3ac

^{1}H NMR ($CDCl_3$, 600 M Hz)



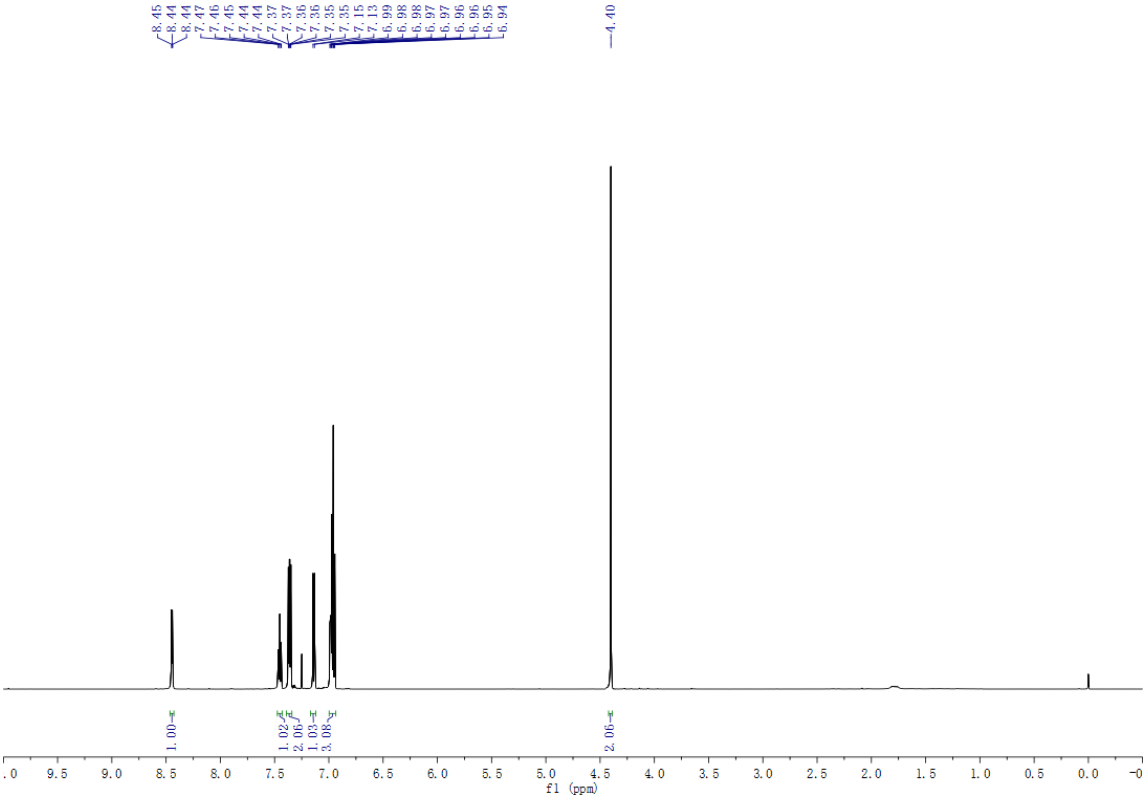
^{13}C NMR ($CDCl_3$, 150 M Hz)



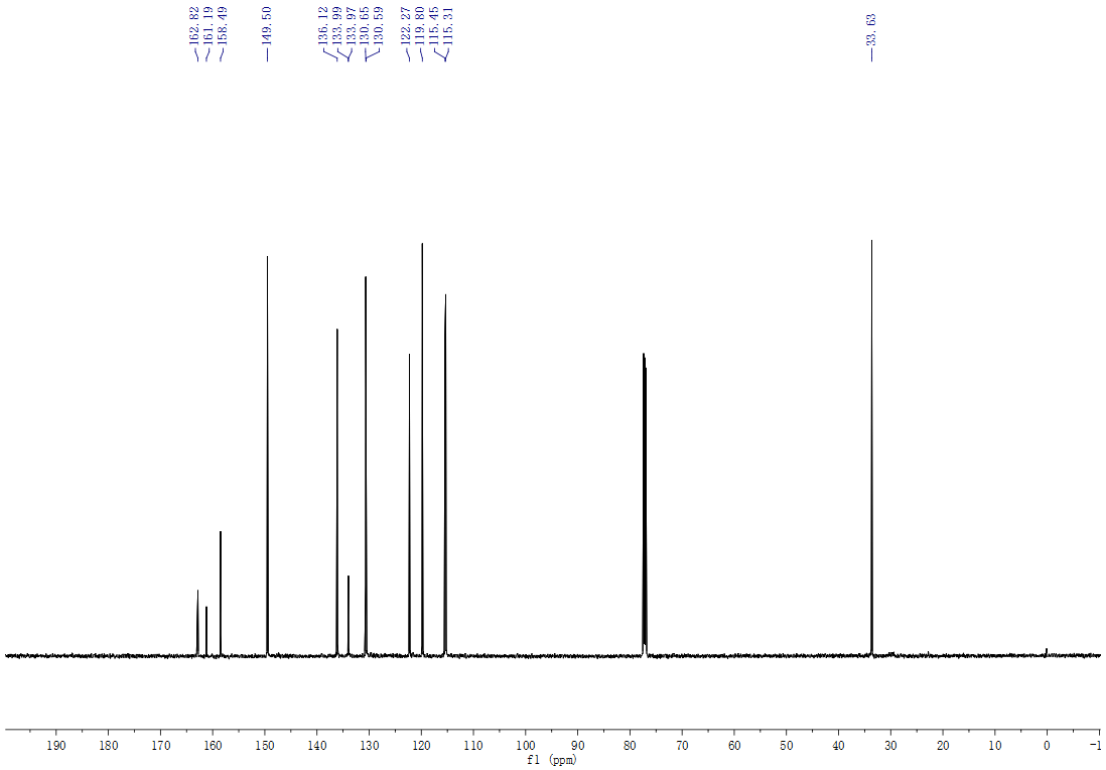


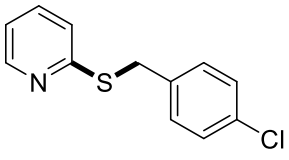
3ad

^{1}H NMR ($CDCl_3$, 600 M Hz)



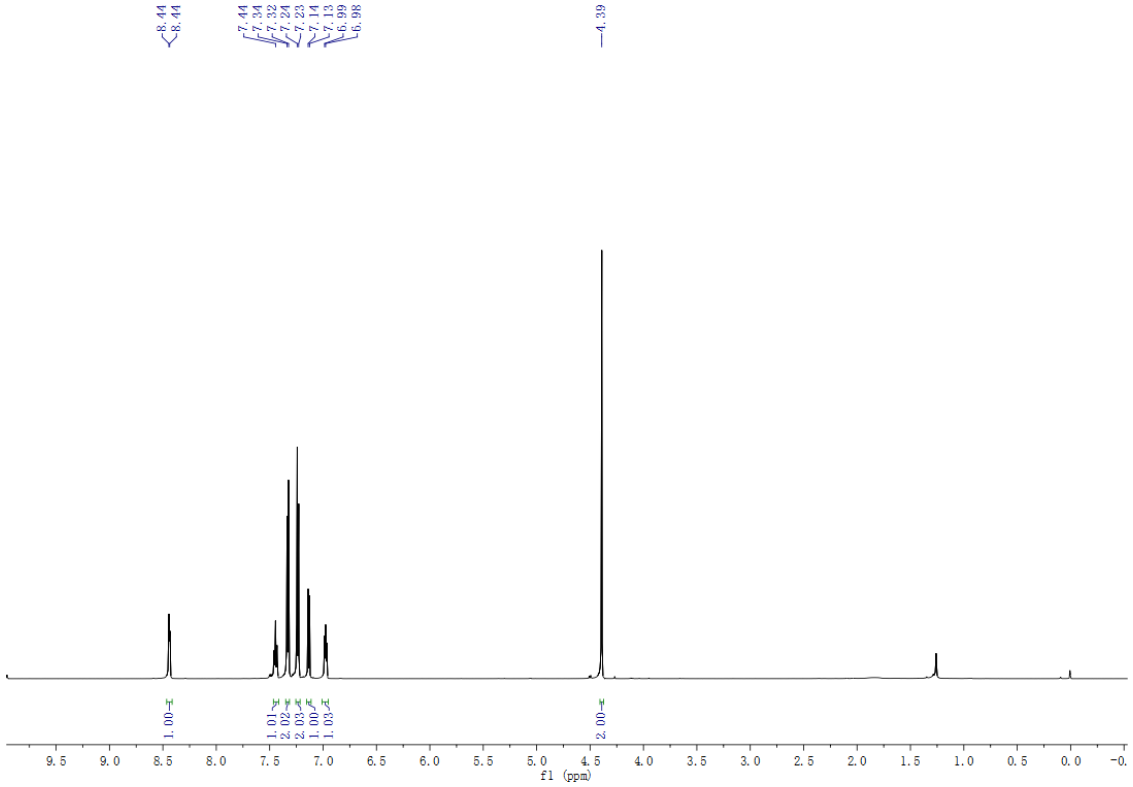
^{13}C NMR ($CDCl_3$, 150 M Hz)



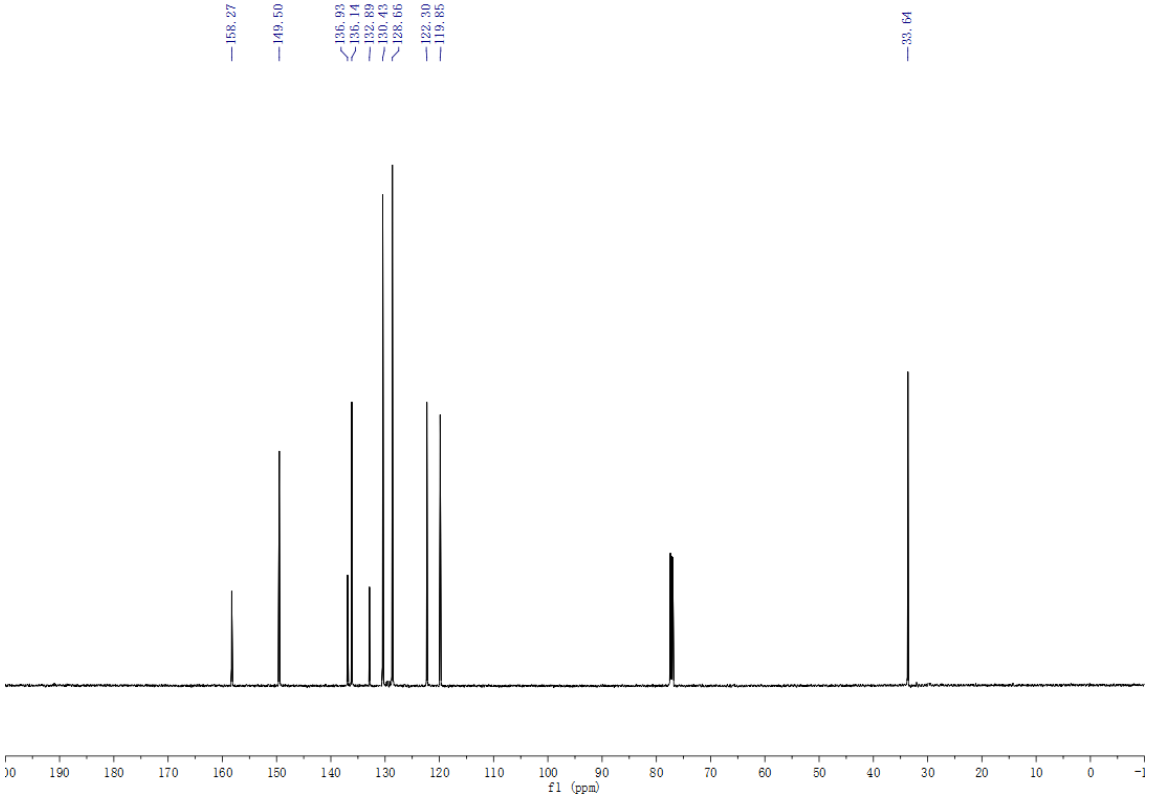


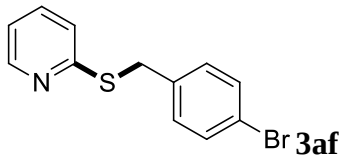
3ae

^{1}H NMR ($CDCl_3$, 600 M Hz)



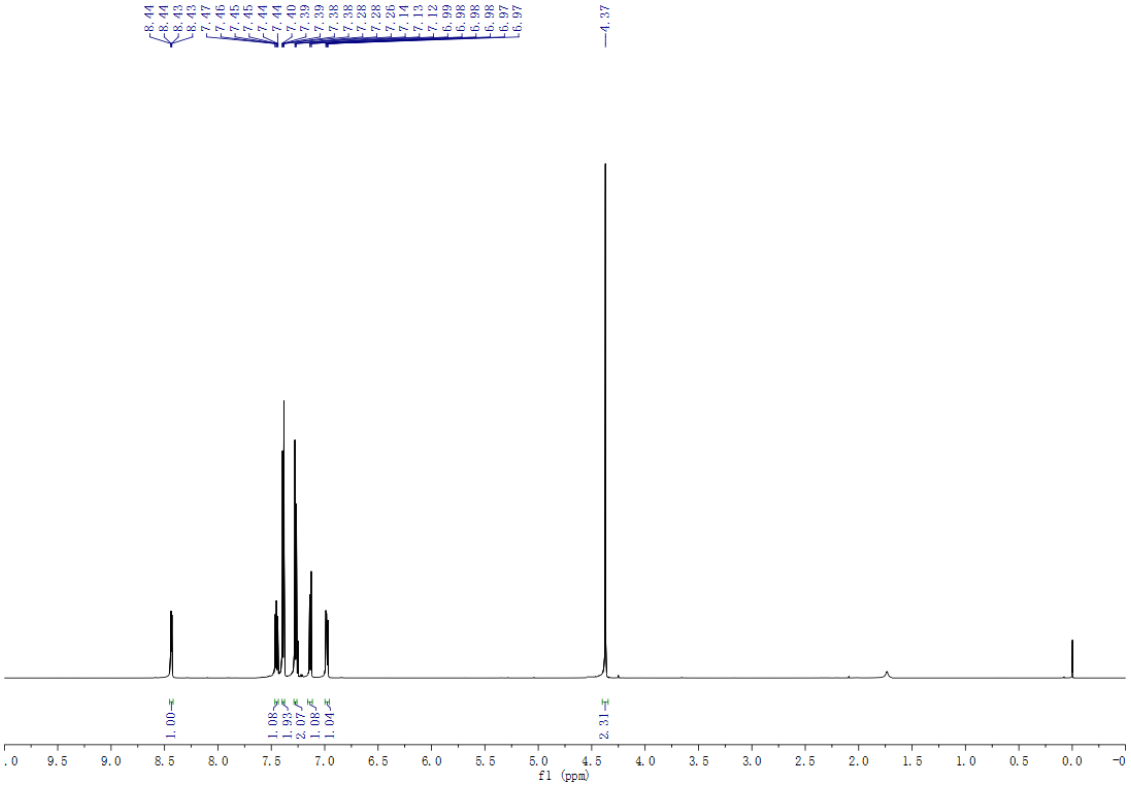
^{13}C NMR ($CDCl_3$, 150 M Hz)



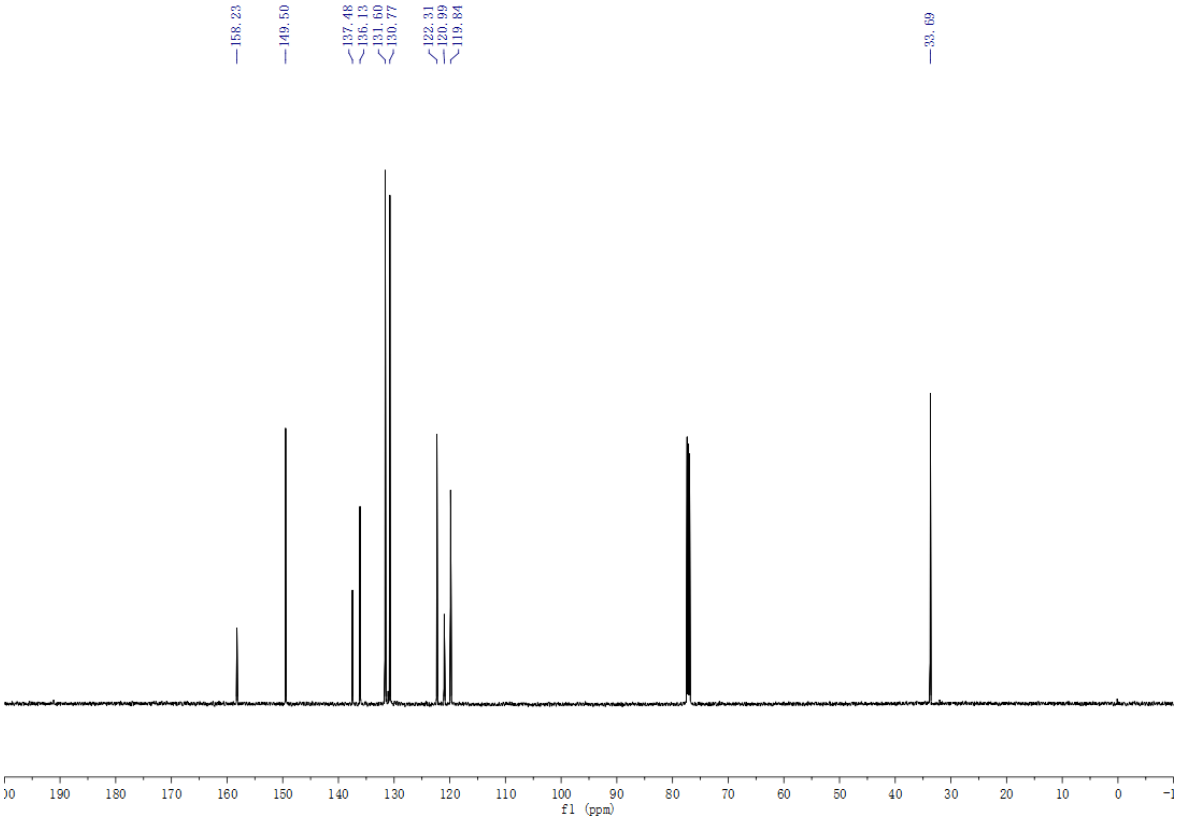


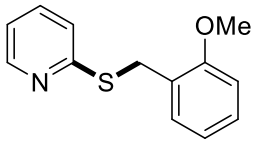
3af

^{1}H NMR ($CDCl_3$, 600 M Hz)



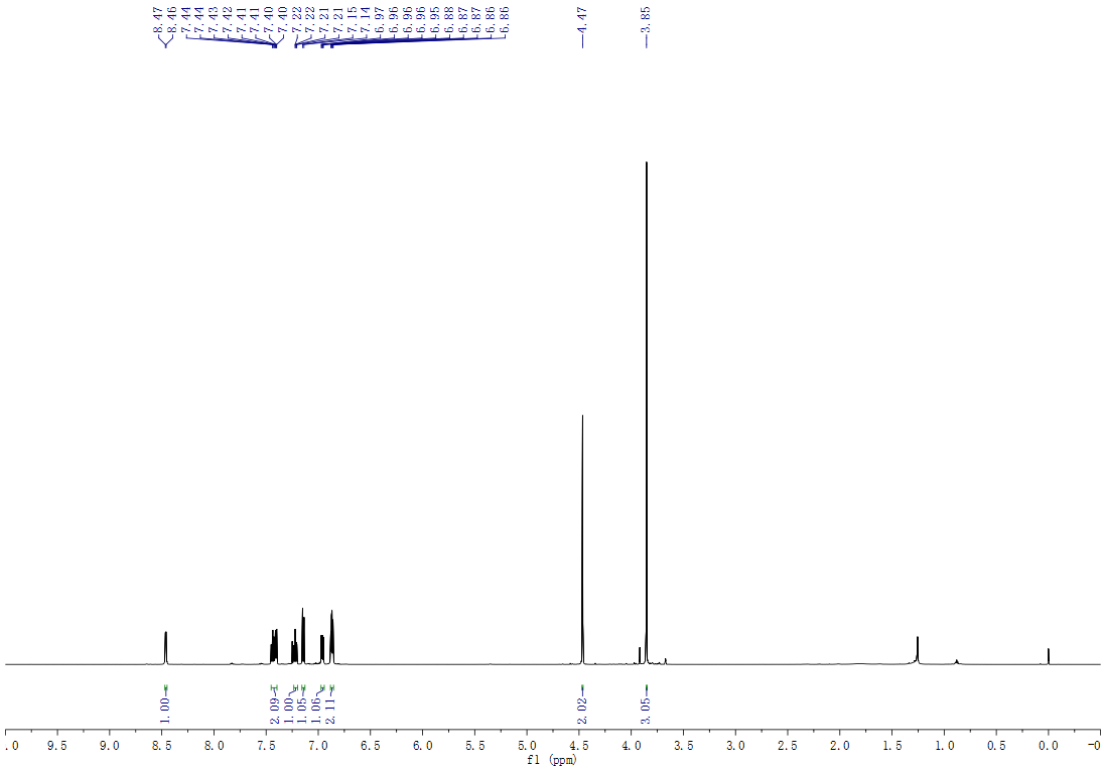
^{13}C NMR ($CDCl_3$, 150 M Hz)



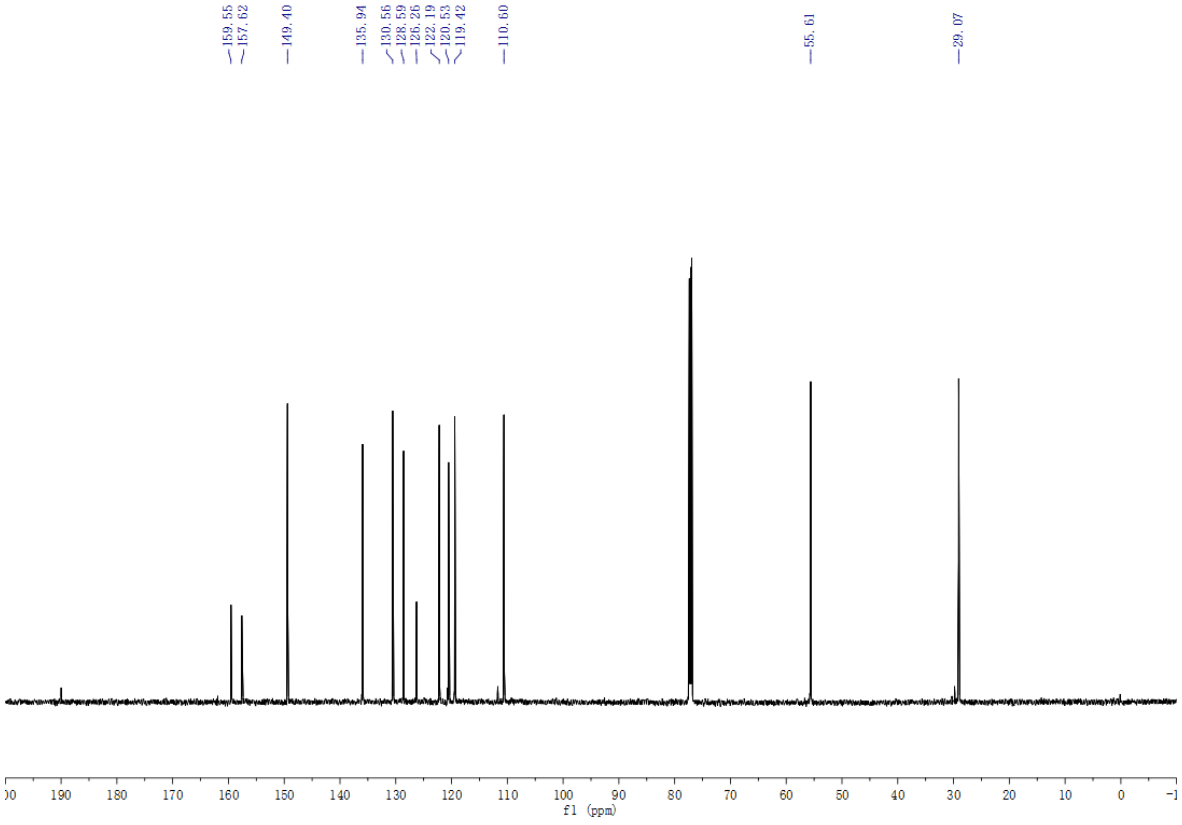


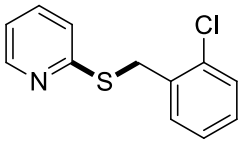
3ag

^{1}H NMR ($CDCl_3$, 600 M Hz)



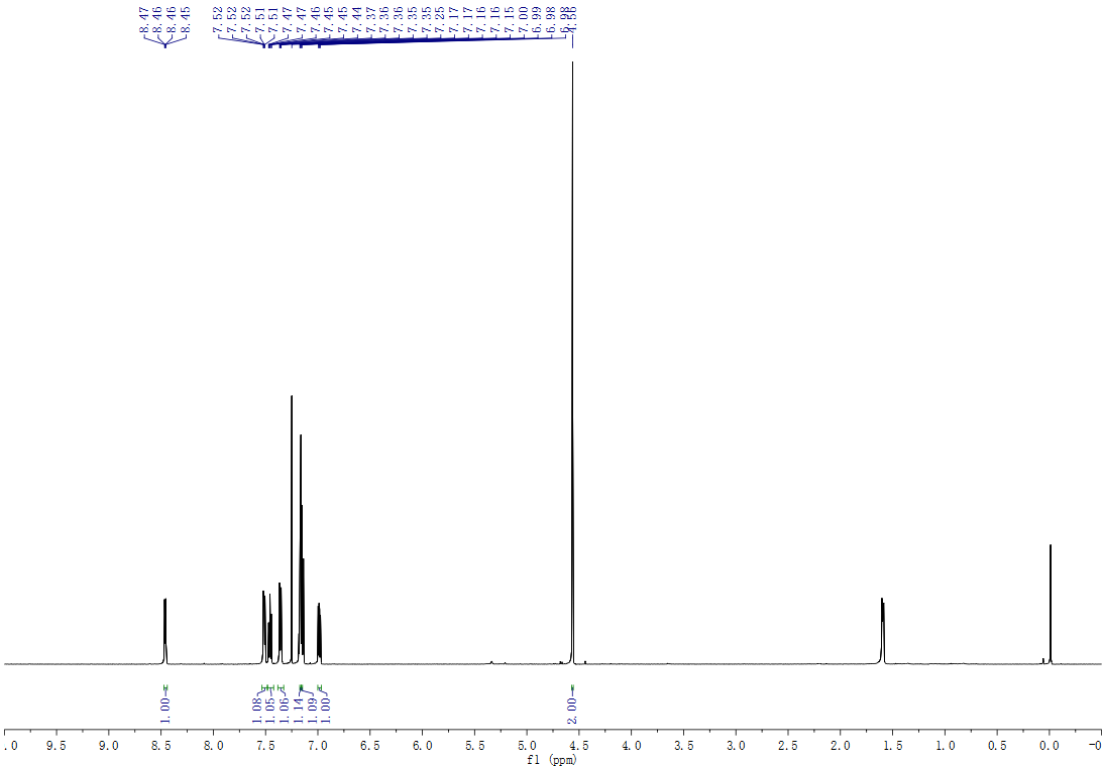
^{13}C NMR ($CDCl_3$, 150 M Hz)



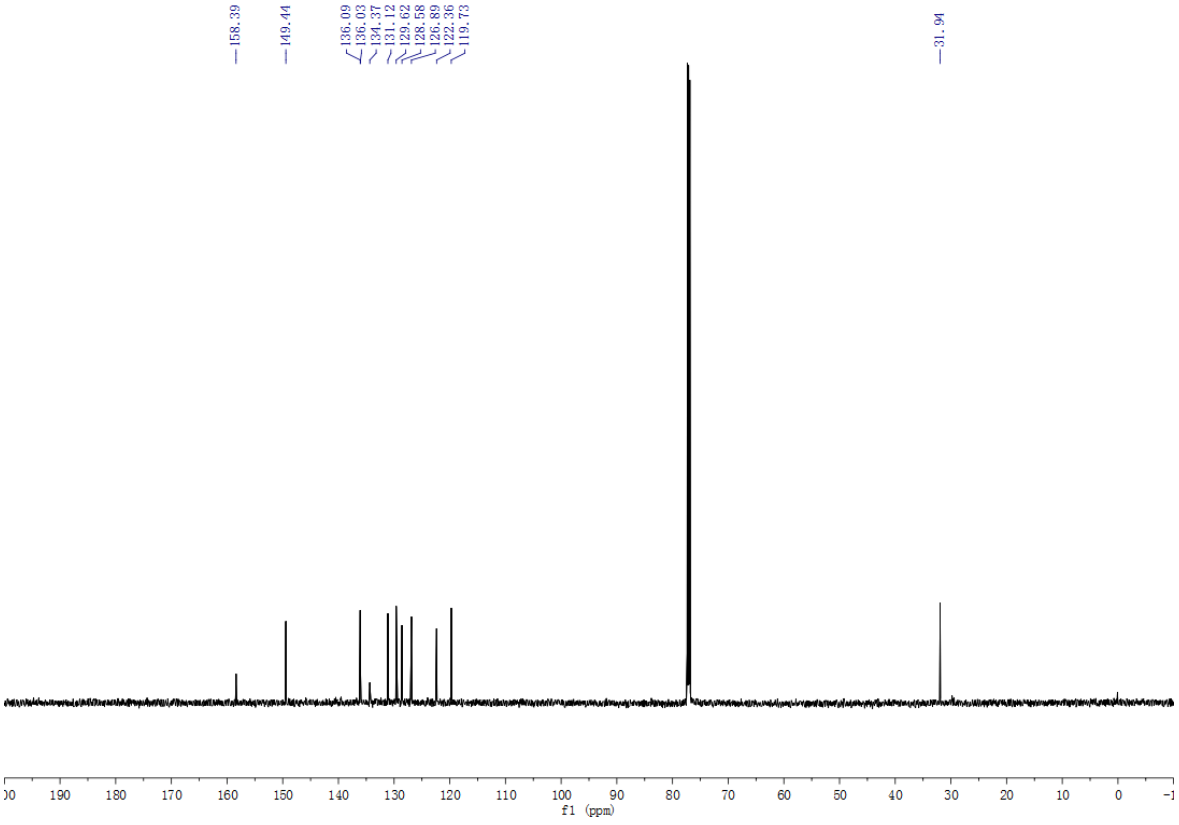


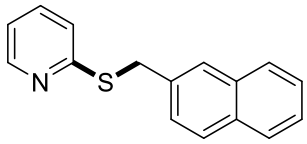
3ah

^{1}H NMR ($CDCl_3$, 600 M Hz)



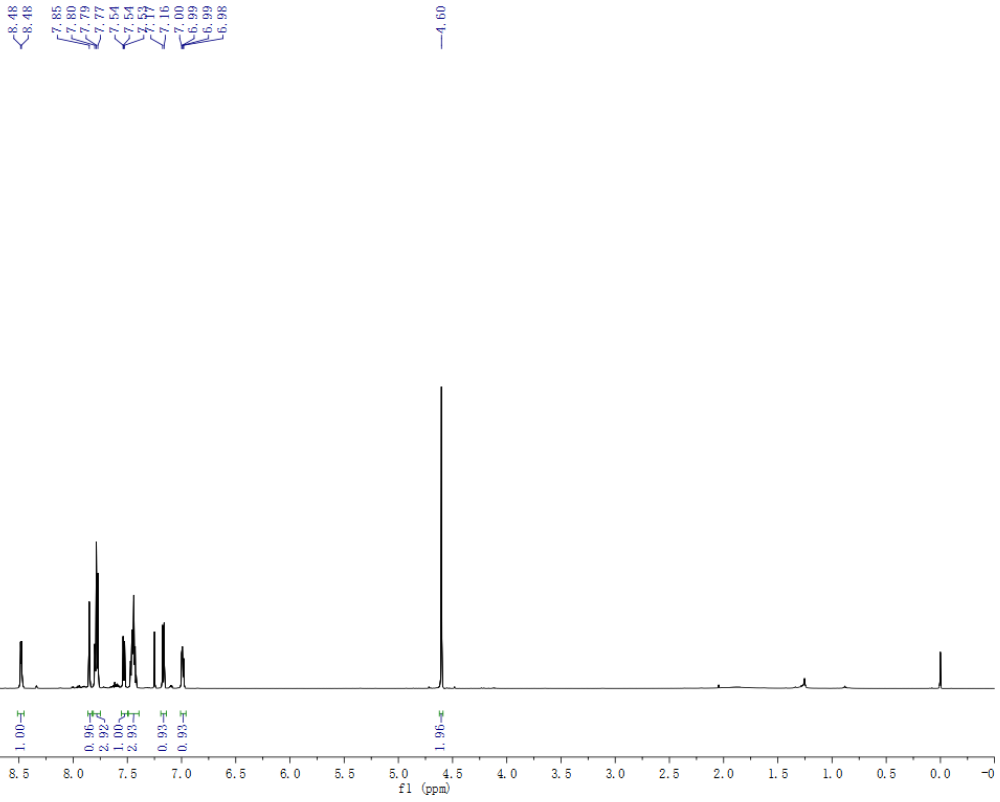
^{13}C NMR ($CDCl_3$, 150 M Hz)



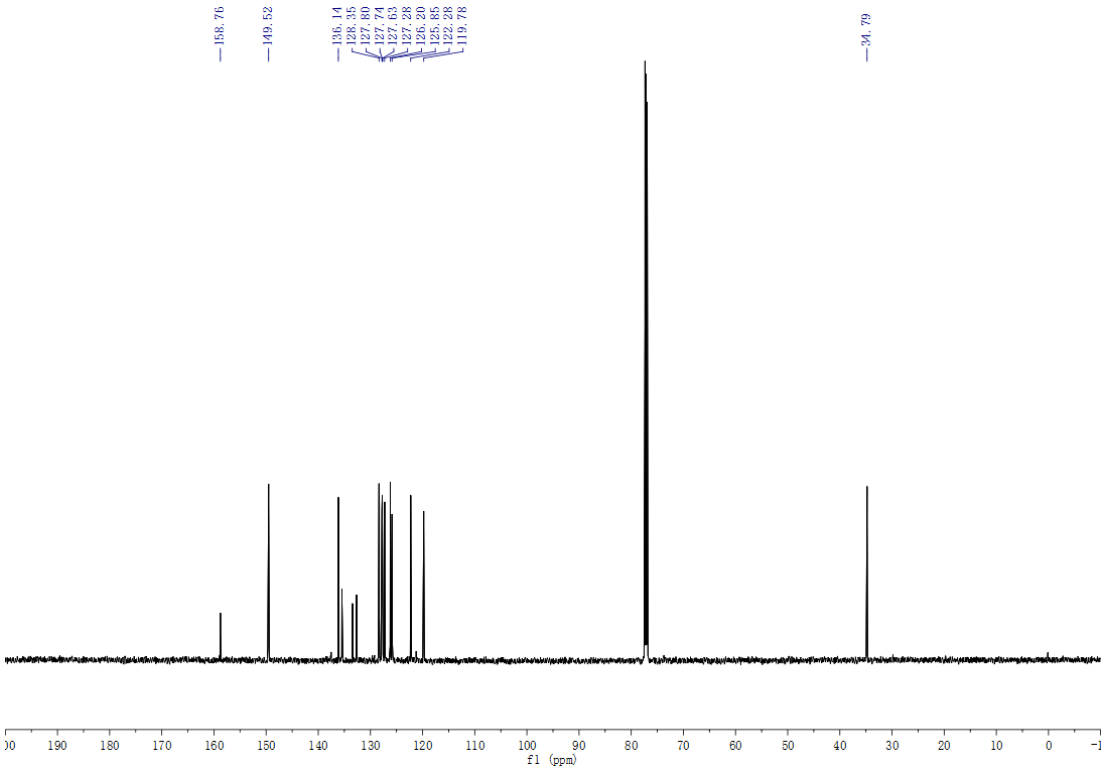


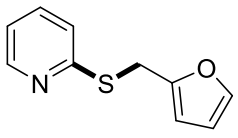
3ai

^{1}H NMR ($CDCl_3$, 600 M Hz)



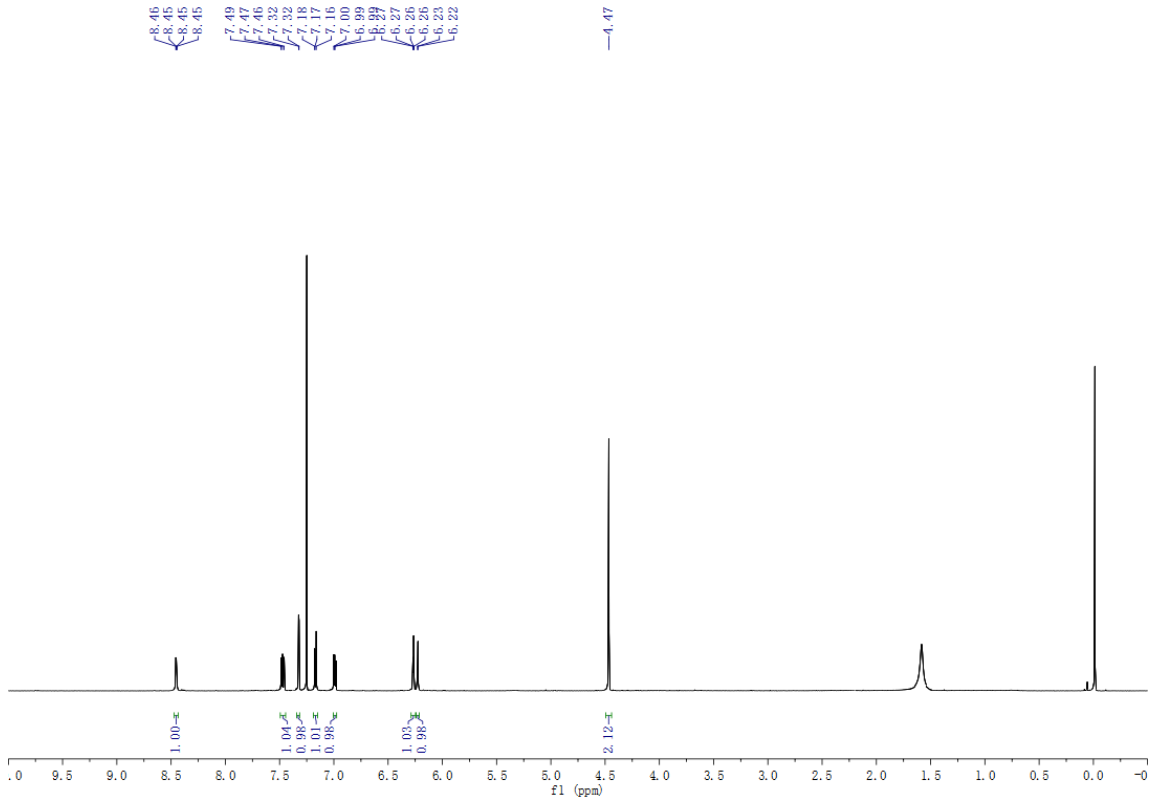
^{13}C NMR ($CDCl_3$, 150 M Hz)



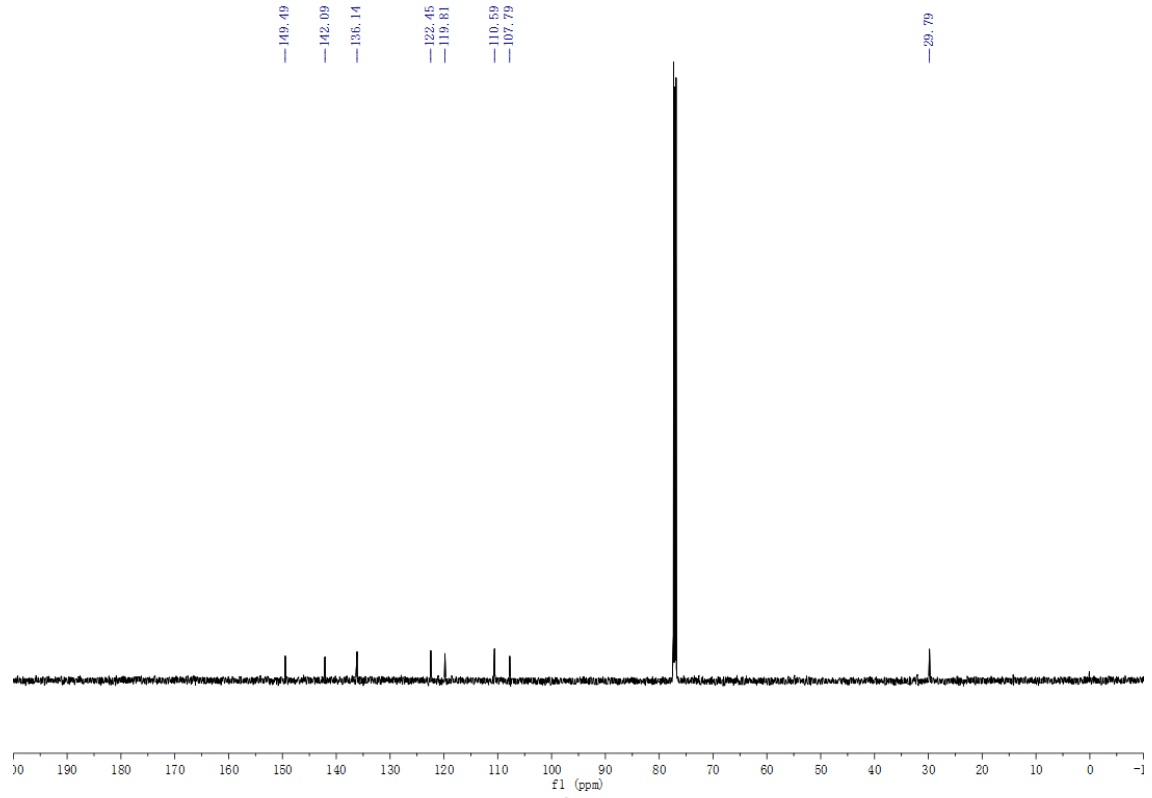


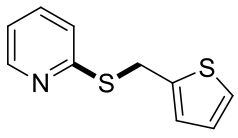
3aj

^{1}H NMR ($CDCl_3$, 600 M Hz)



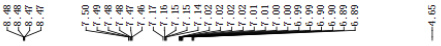
^{13}C NMR ($CDCl_3$, 150 M Hz)

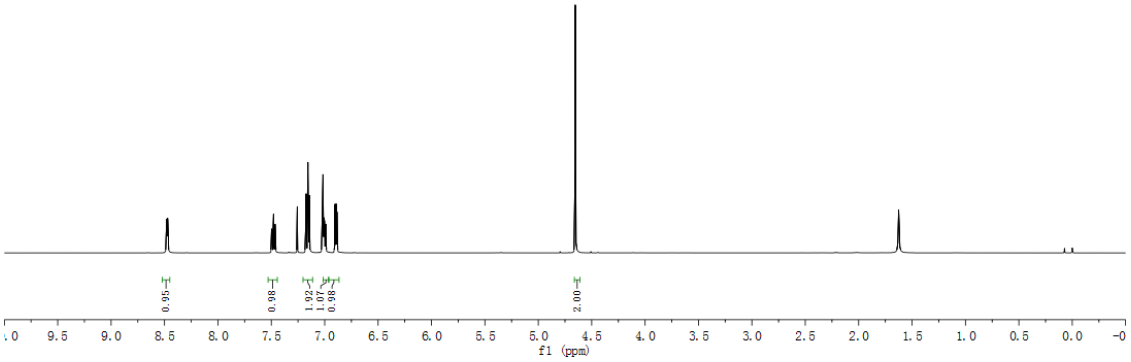




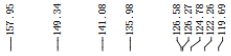
3ak

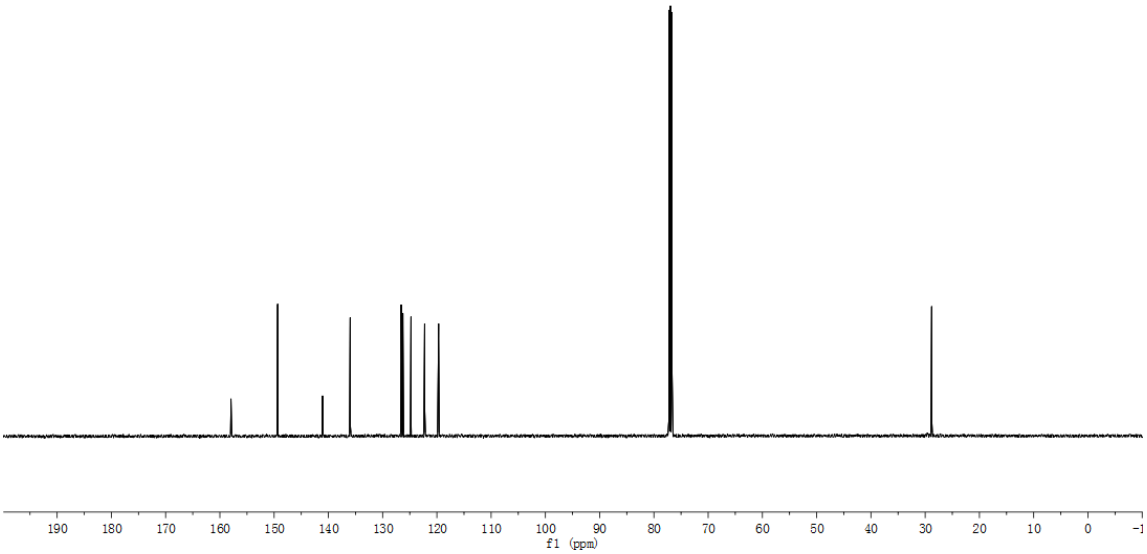
^{1}H NMR ($CDCl_3$, 600M Hz)

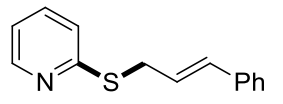




^{13}C NMR ($CDCl_3$, 150 M Hz)

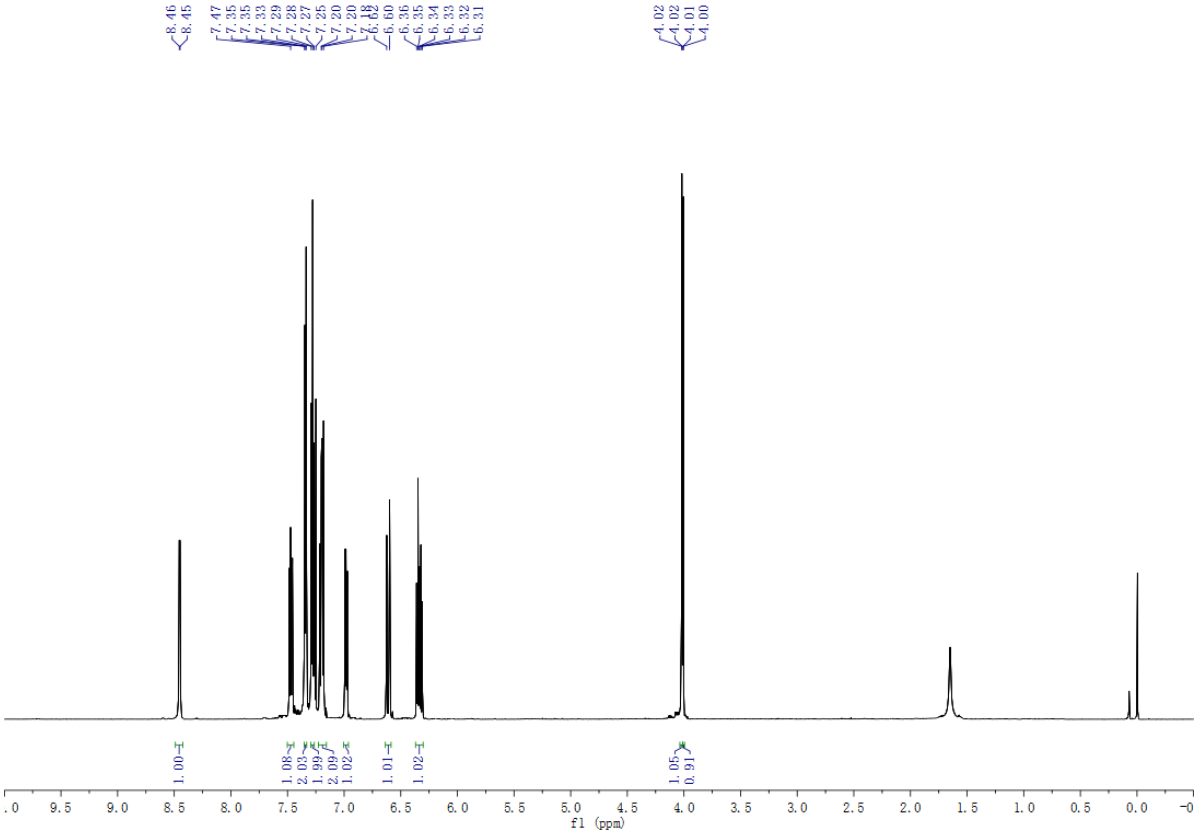




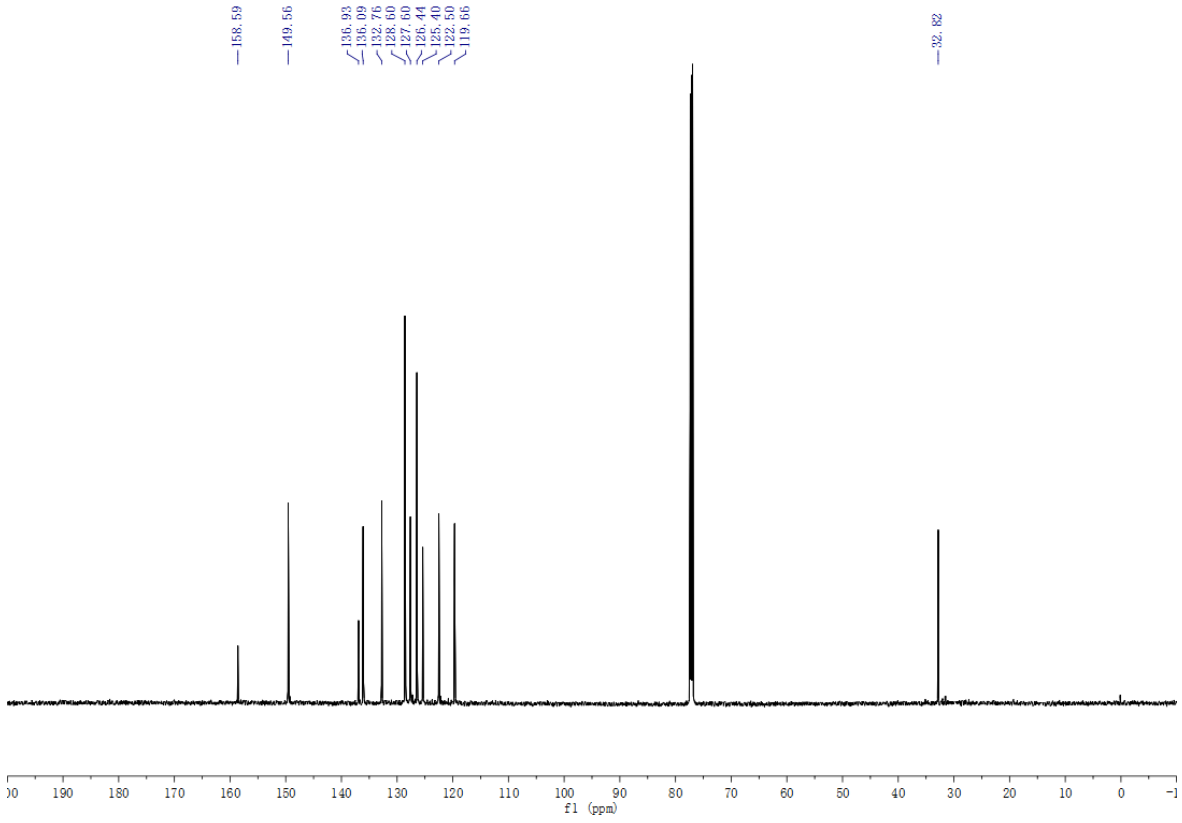


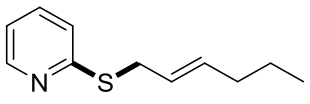
3al

^{1}H NMR ($CDCl_3$, 600 M Hz)



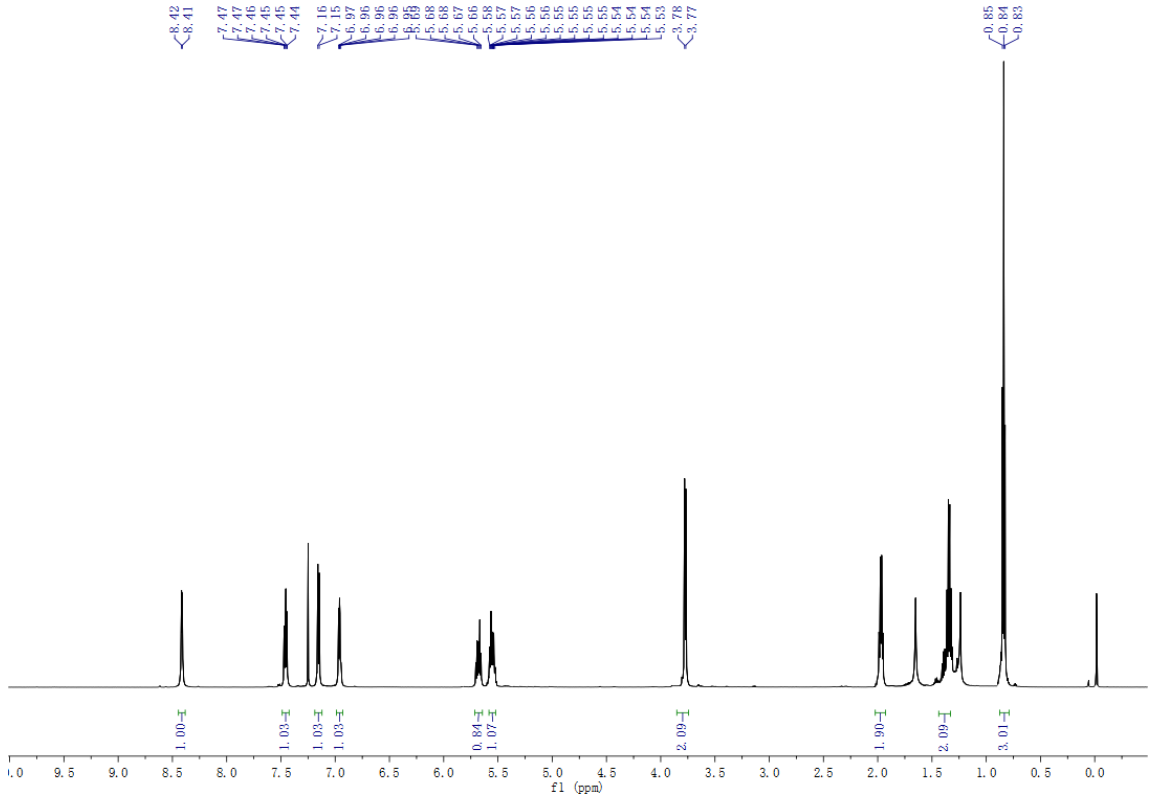
^{13}C NMR ($CDCl_3$, 150 M Hz)



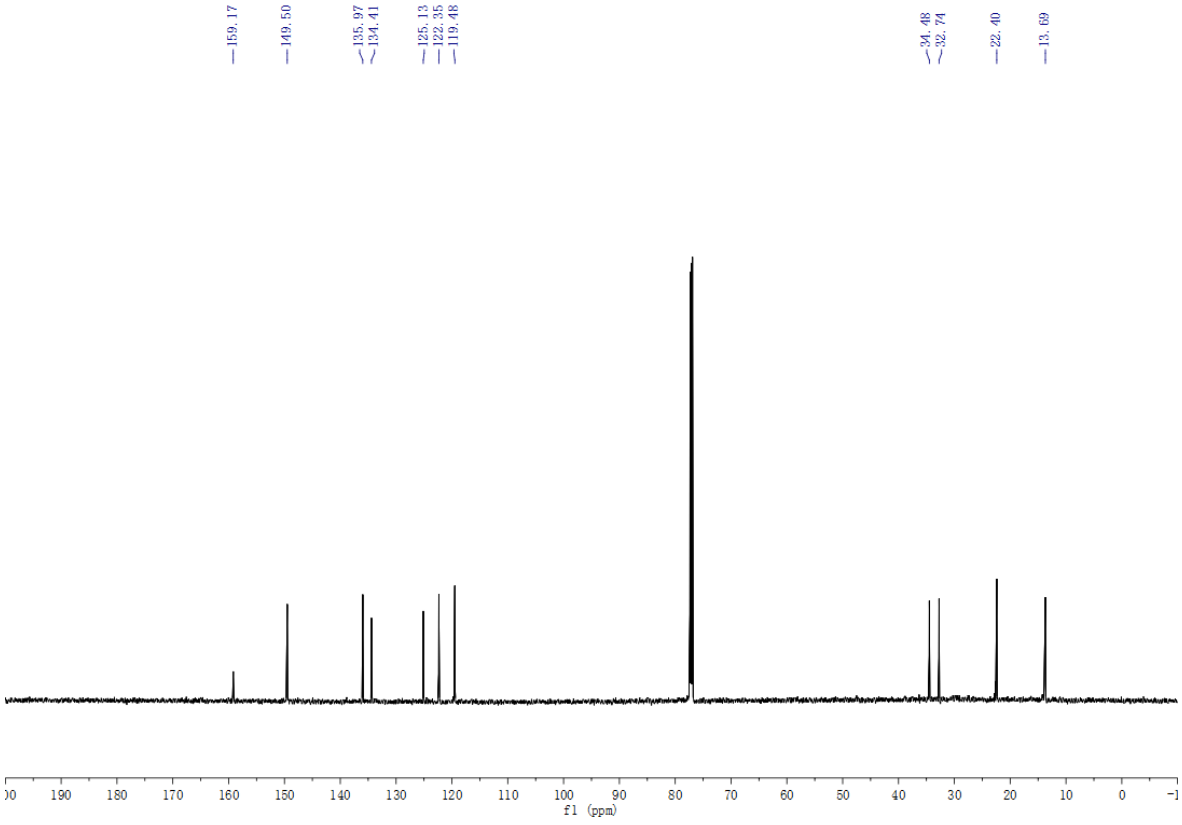


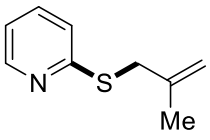
3am

^{1}H NMR ($CDCl_3$, 600 M Hz)



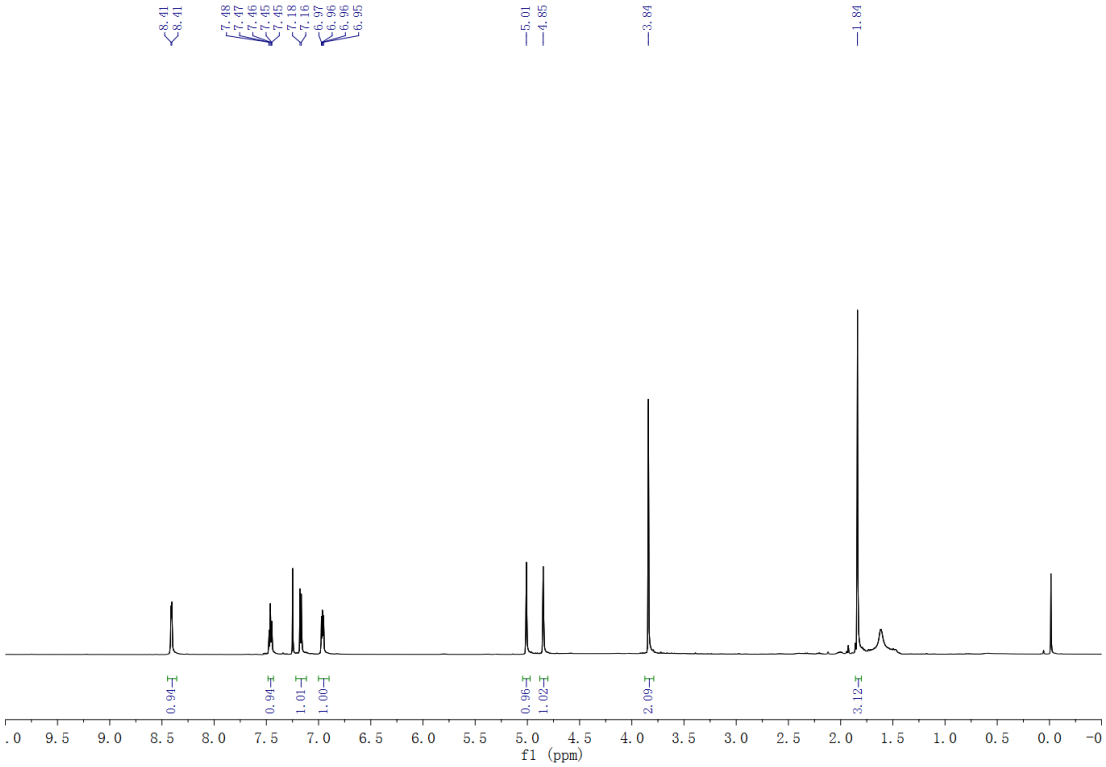
^{13}C NMR ($CDCl_3$, 150 M Hz)



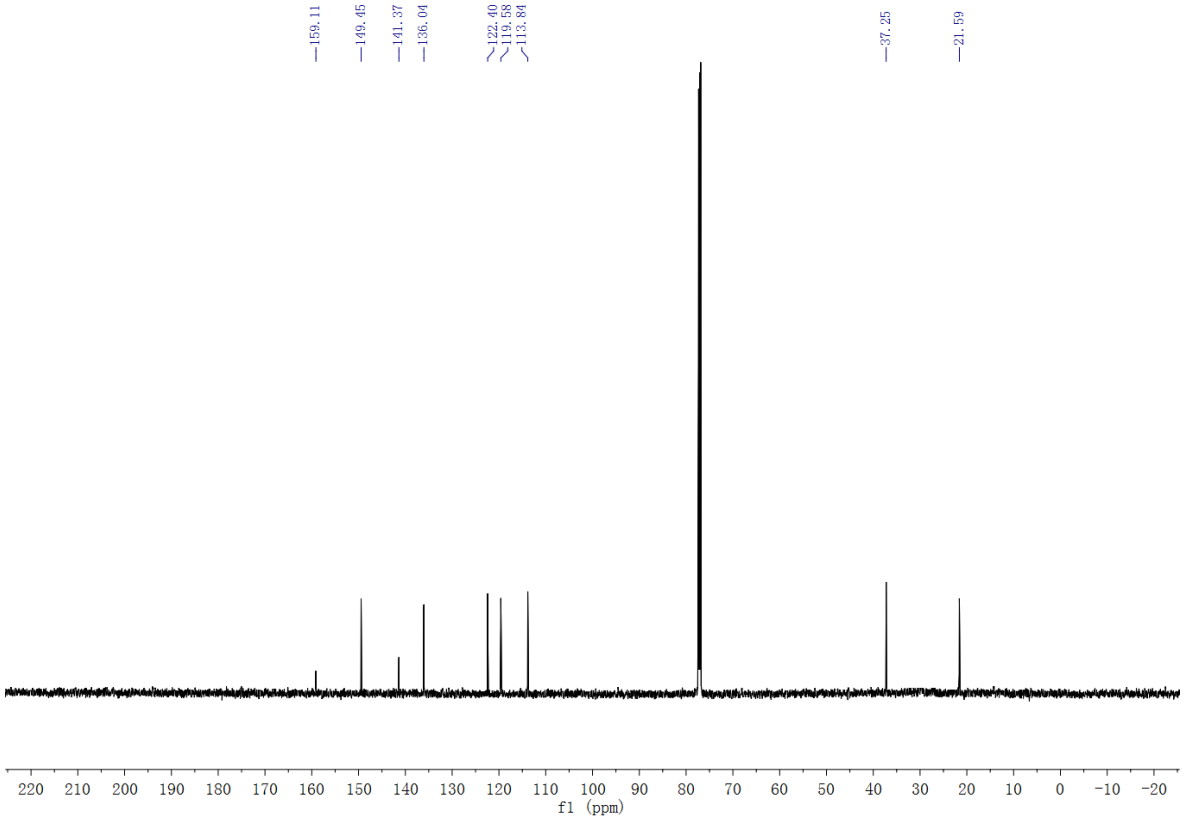


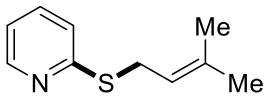
3an

^{1}H NMR ($CDCl_3$, 600 M Hz)



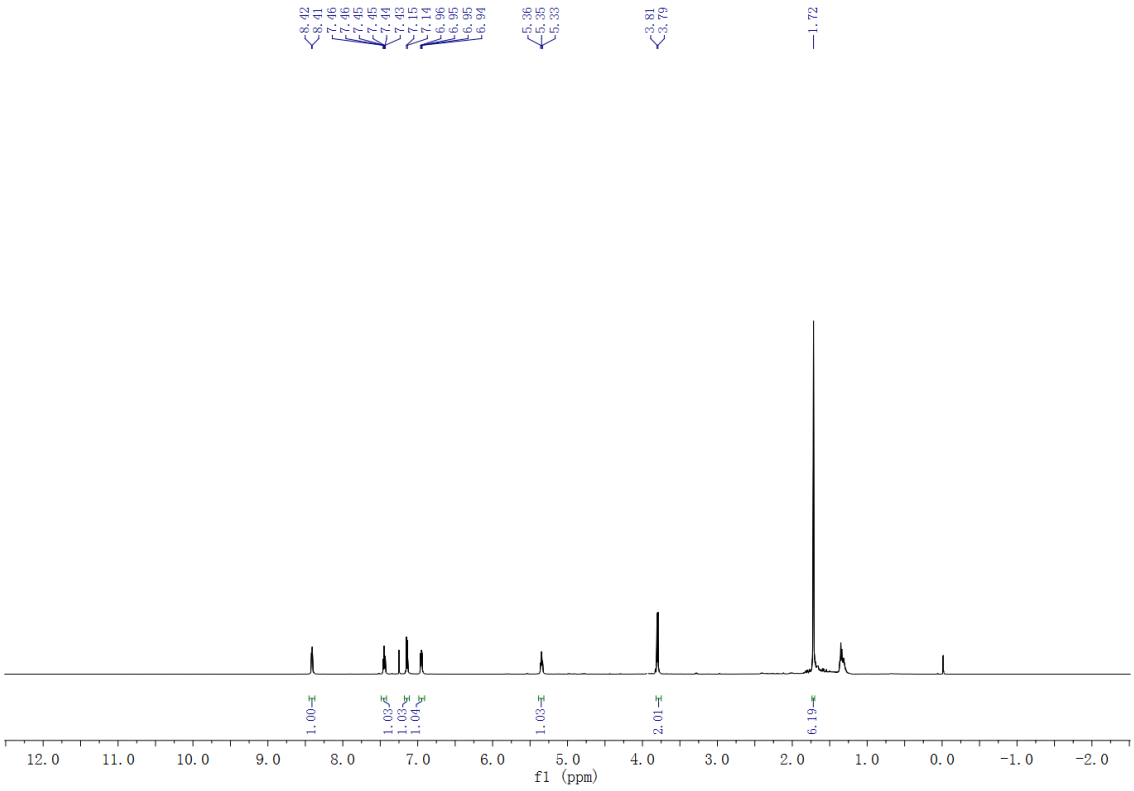
^{13}C NMR ($CDCl_3$, 150 M Hz)



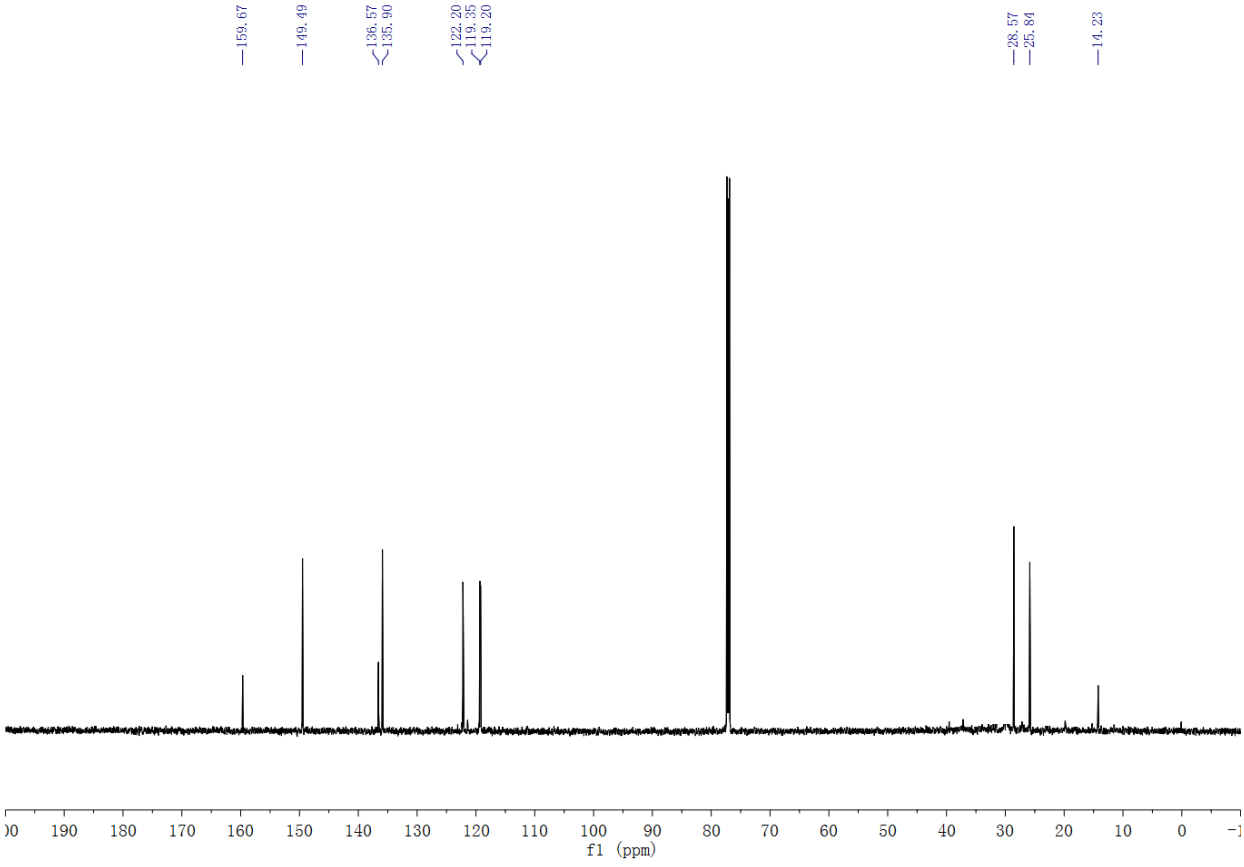


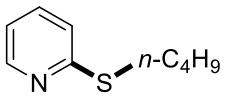
3ao

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)





3ap

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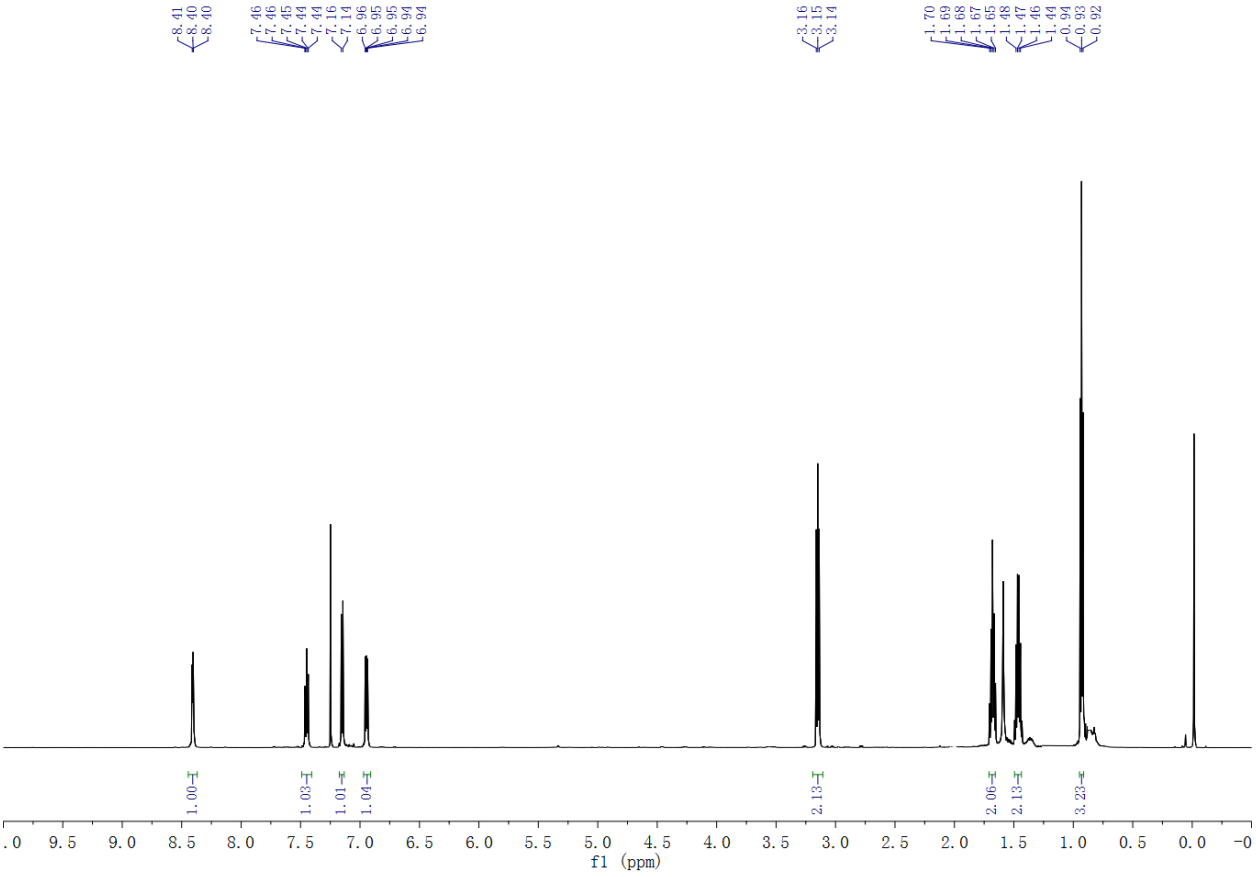
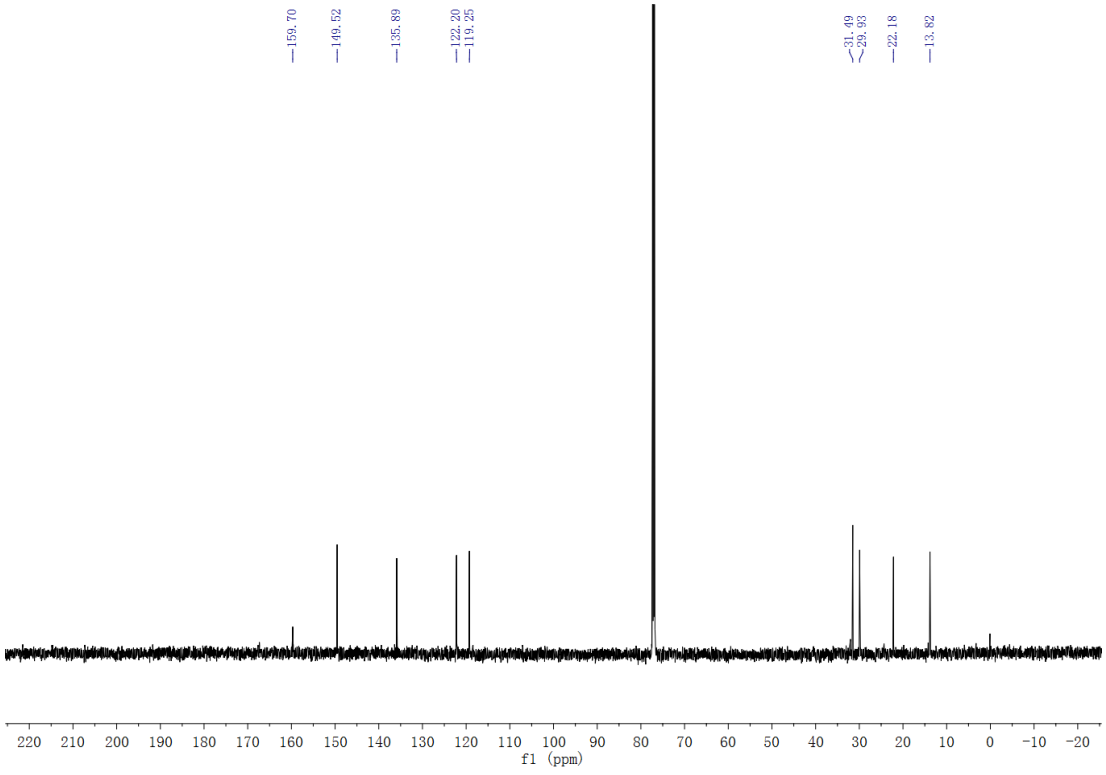
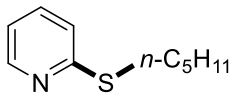


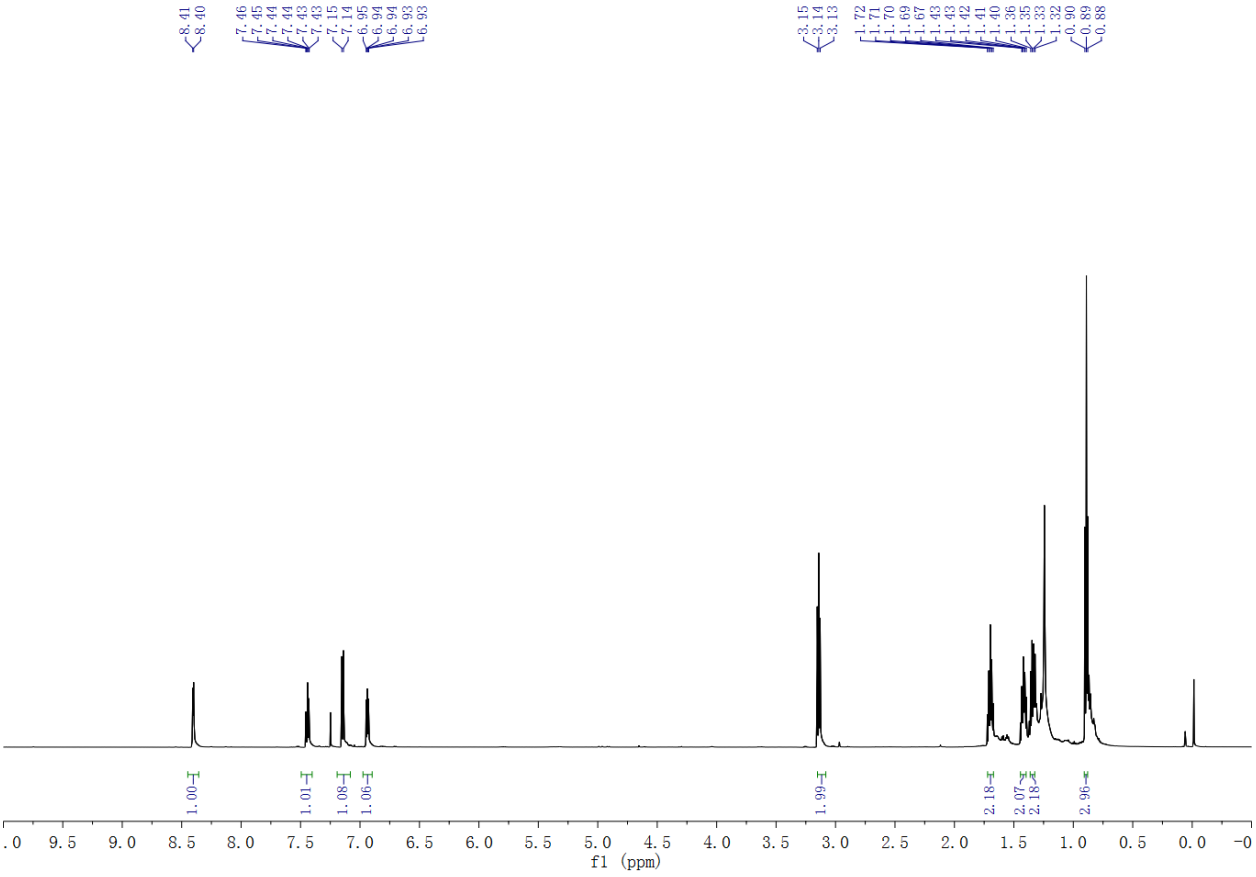
^{13}C NMR ($CDCl_3$, 150 M Hz)



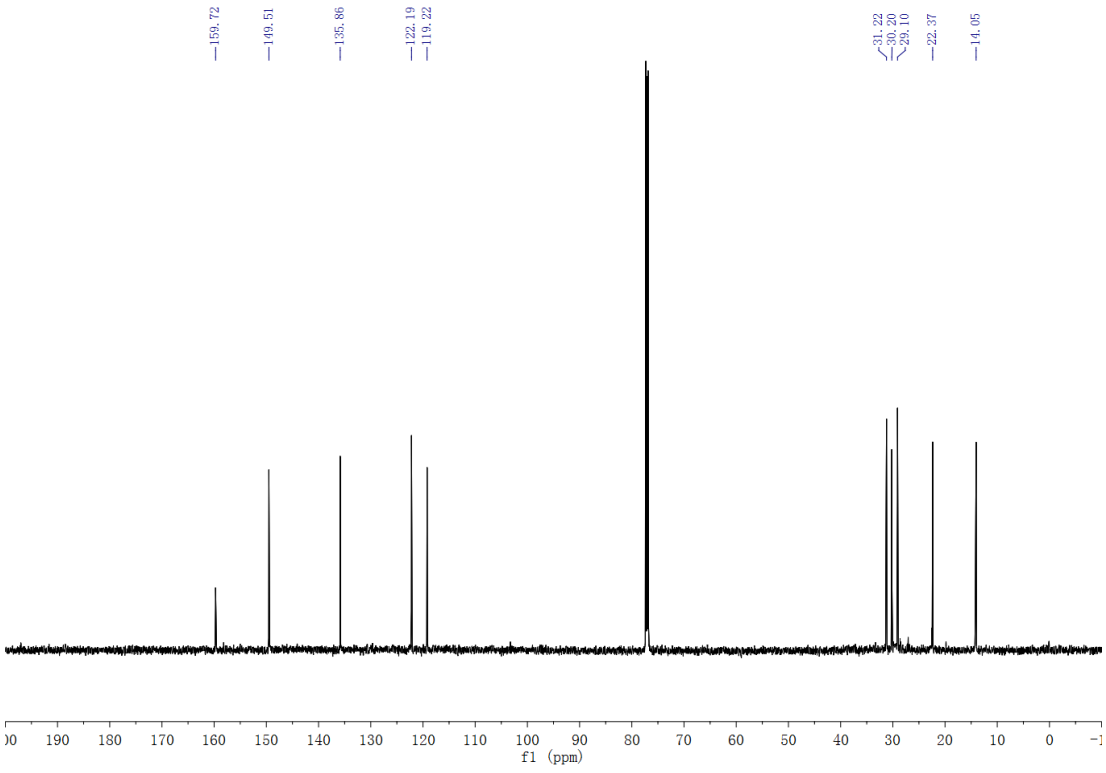


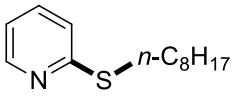
3aq

^{1}H NMR ($CDCl_3$, 600 M Hz)



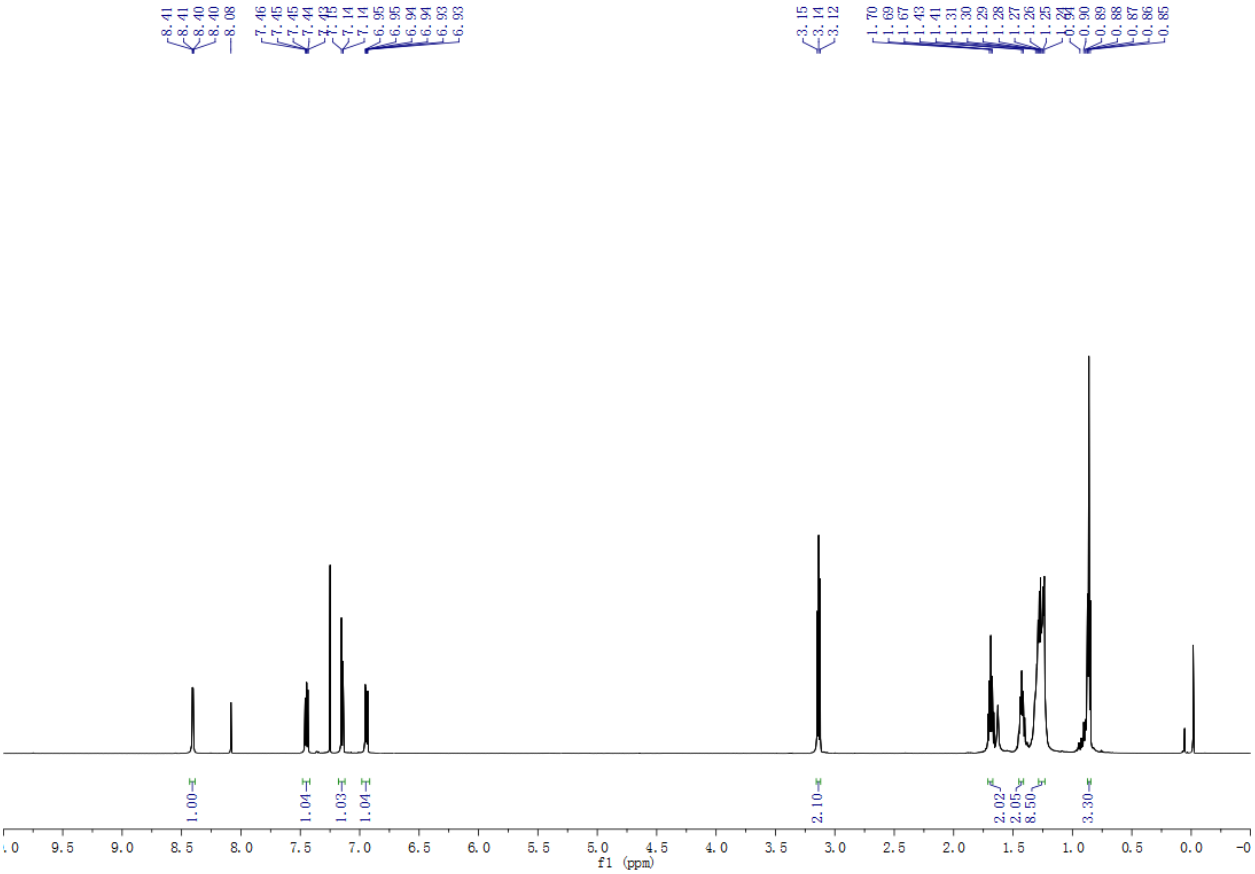
^{13}C NMR ($CDCl_3$, 150 M Hz)



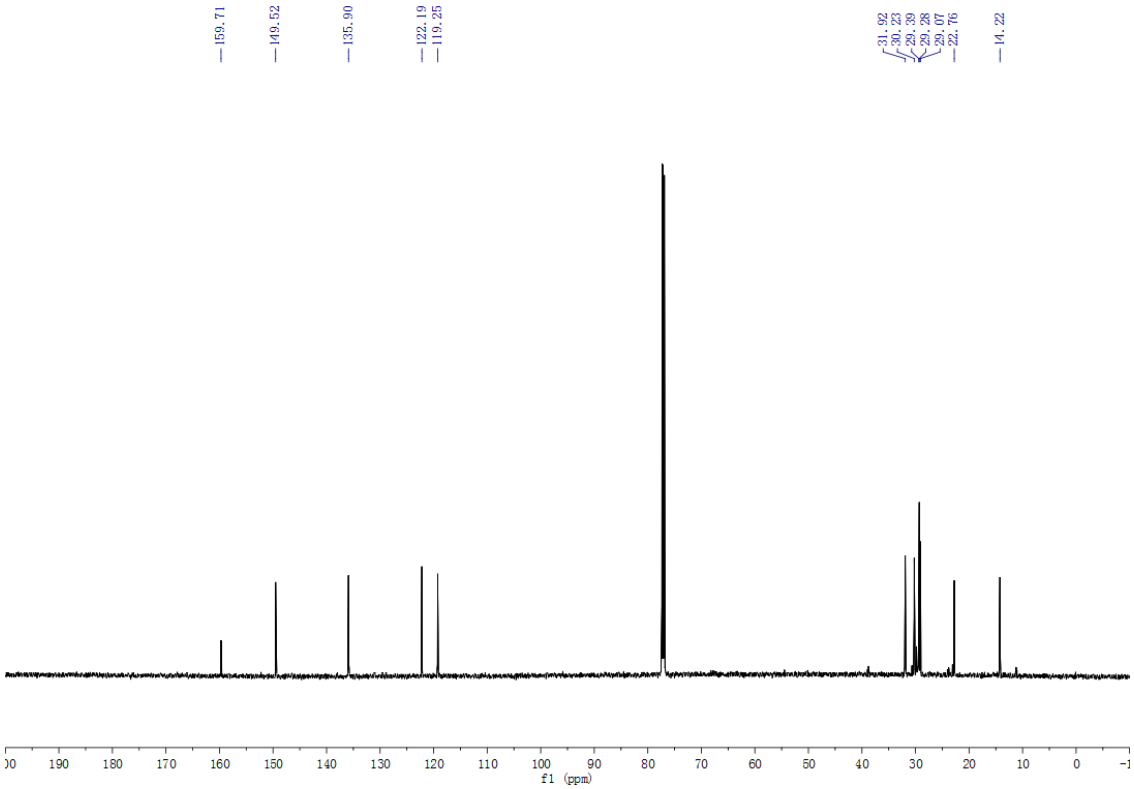


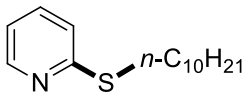
3ar

^{1}H NMR ($CDCl_3$, 600 M Hz)



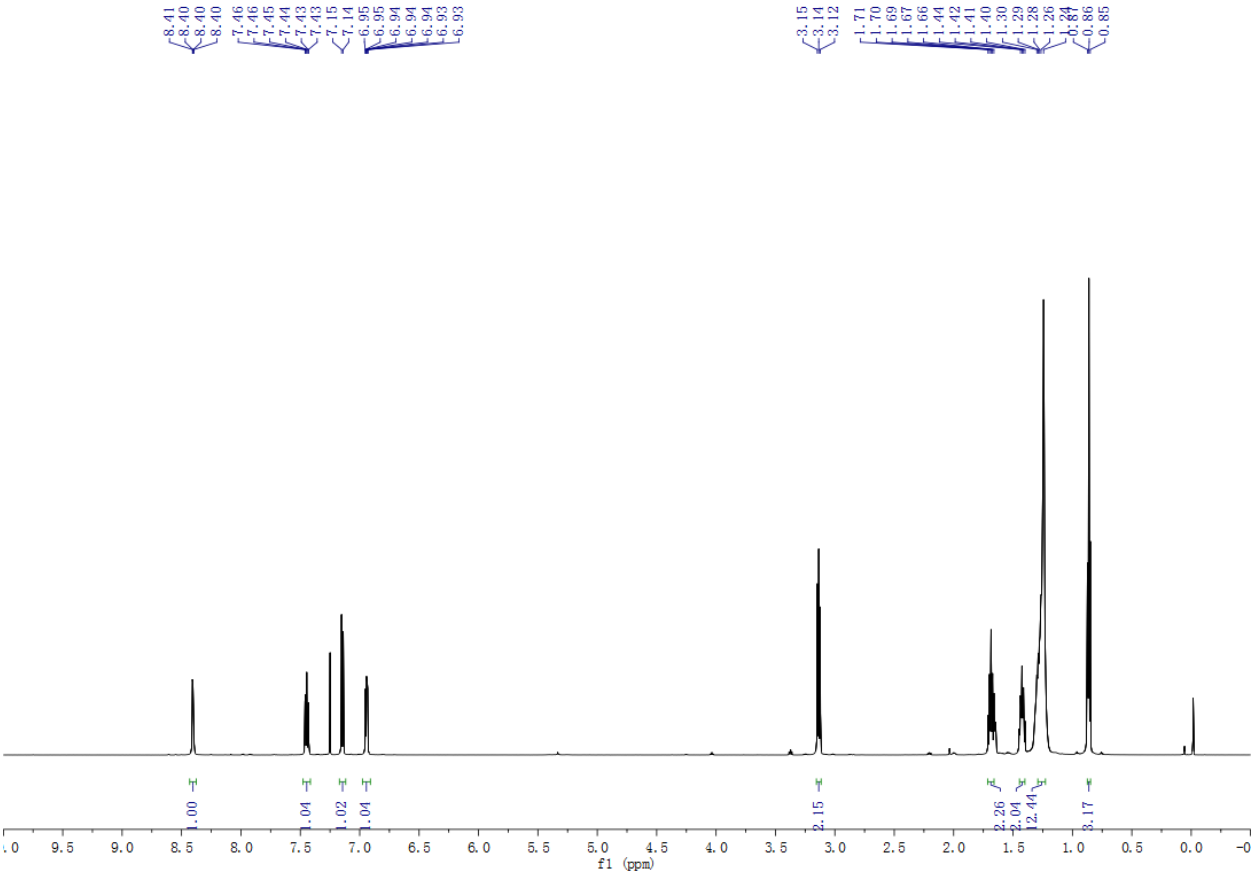
^{13}C NMR ($CDCl_3$, 150 M Hz)



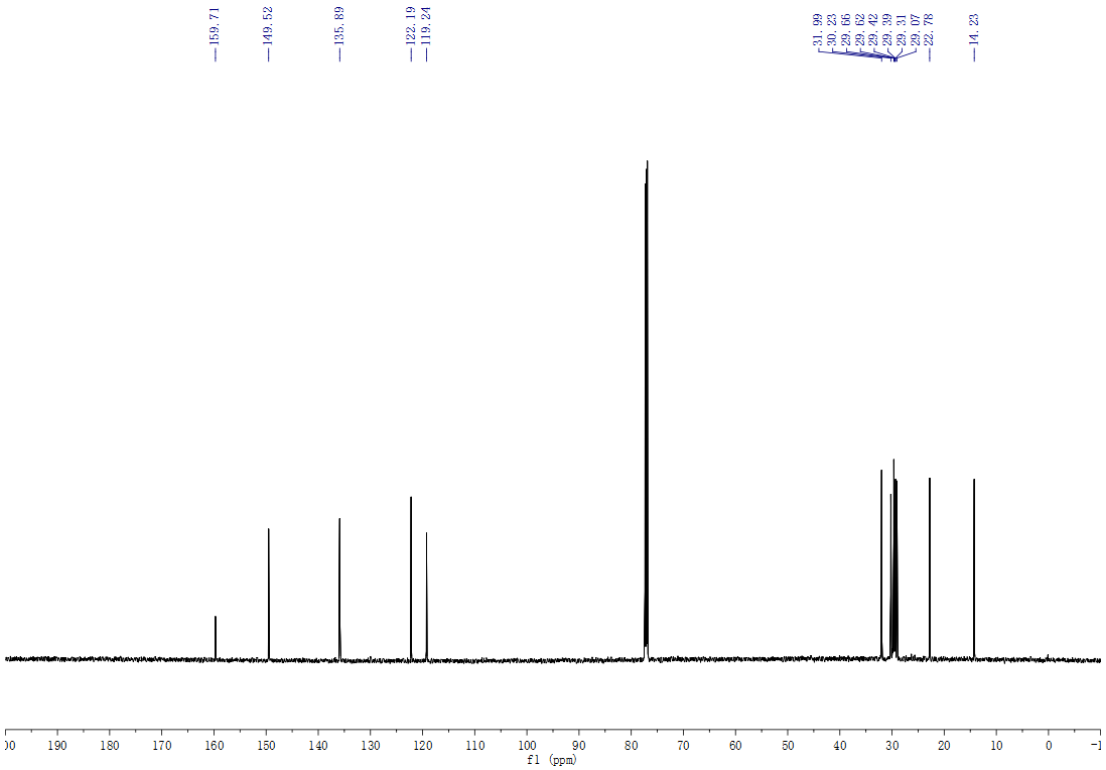


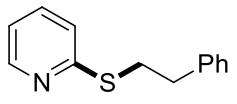
3as

^{1}H NMR ($CDCl_3$, 600 M Hz)



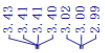
^{13}C NMR ($CDCl_3$, 150 M Hz)

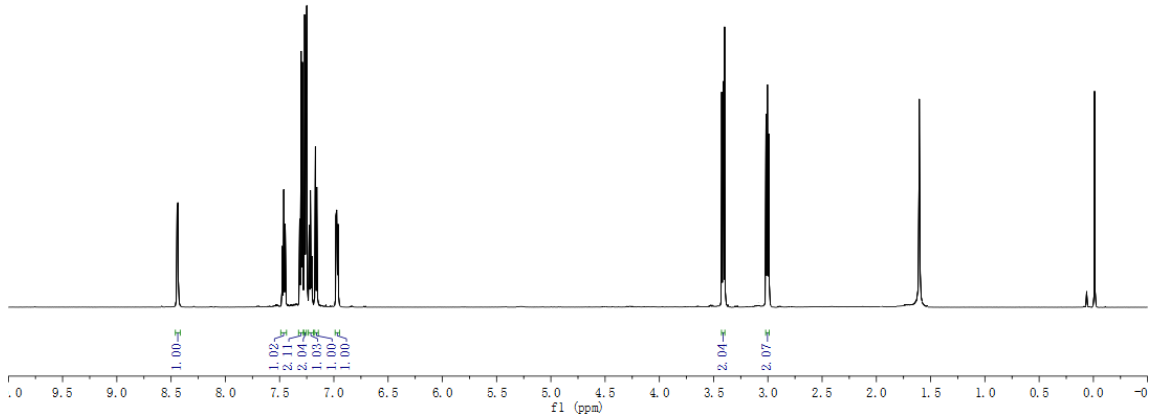




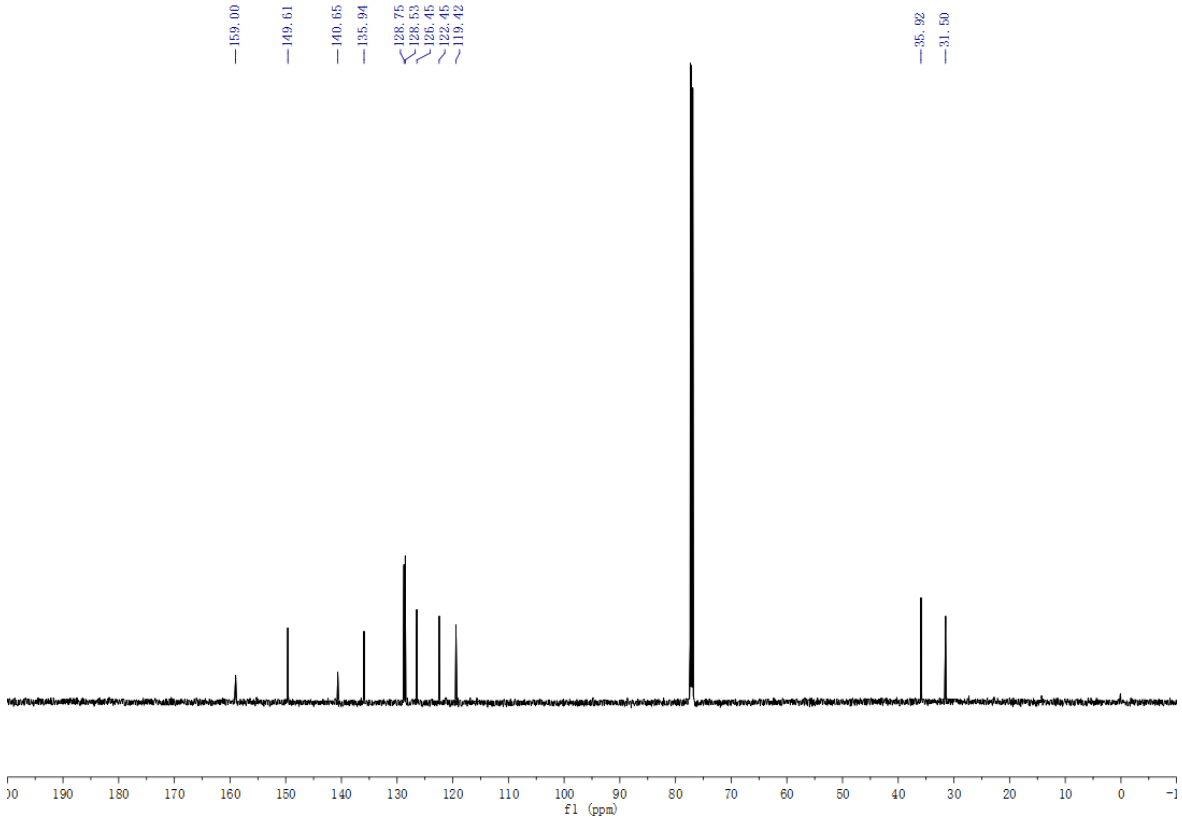
3at

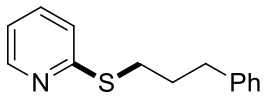
^{1}H NMR ($CDCl_3$, 600 M Hz)





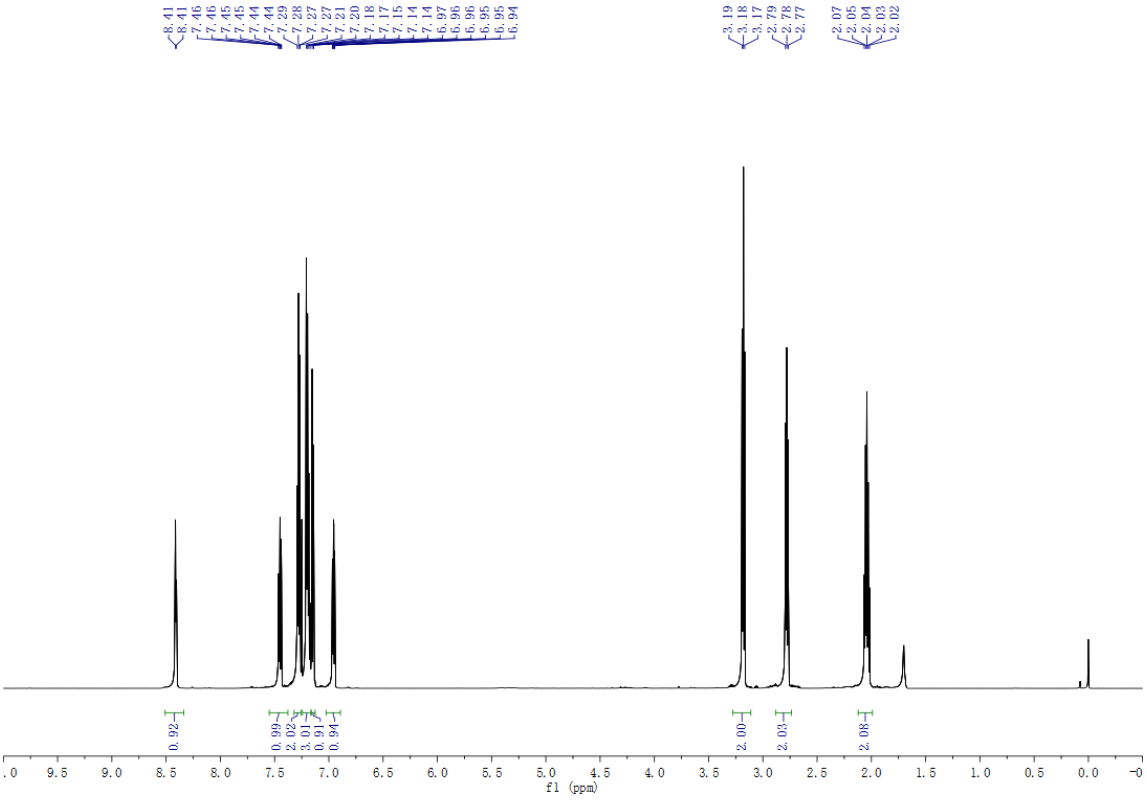
^{13}C NMR ($CDCl_3$, 150 M Hz)



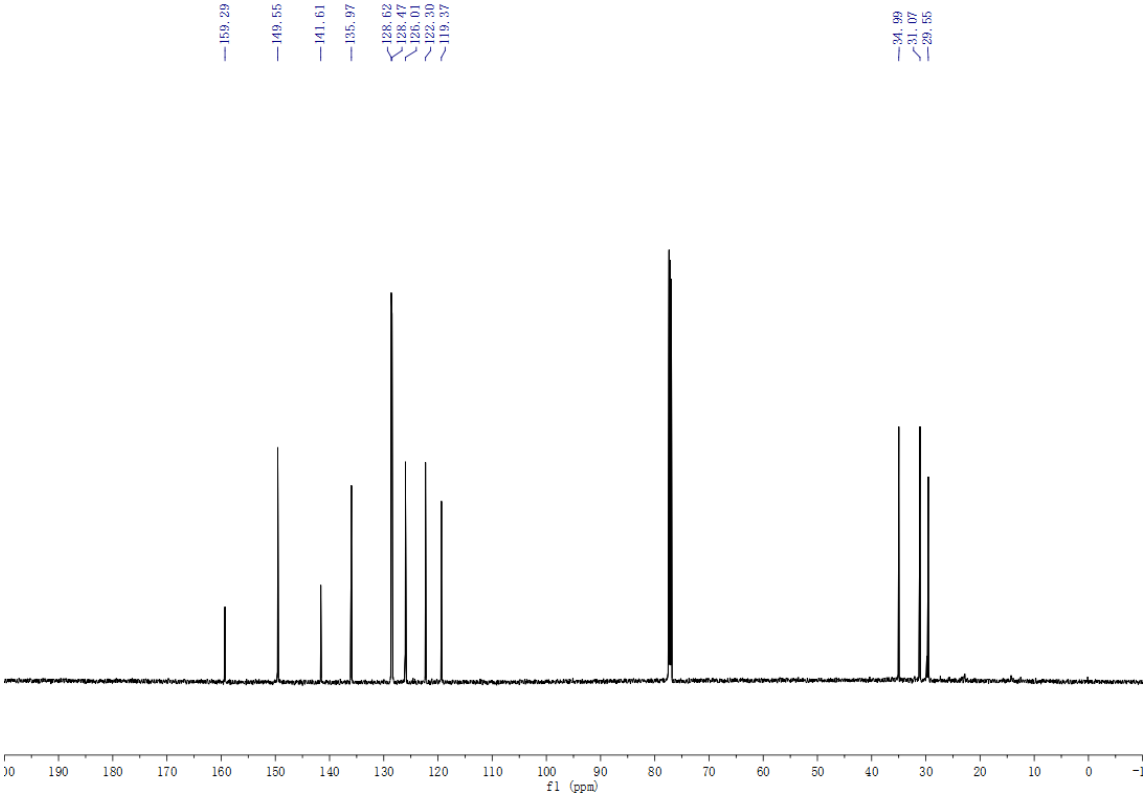


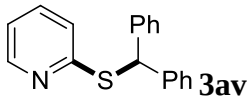
3au

^{1}H NMR ($CDCl_3$, 600 M Hz)



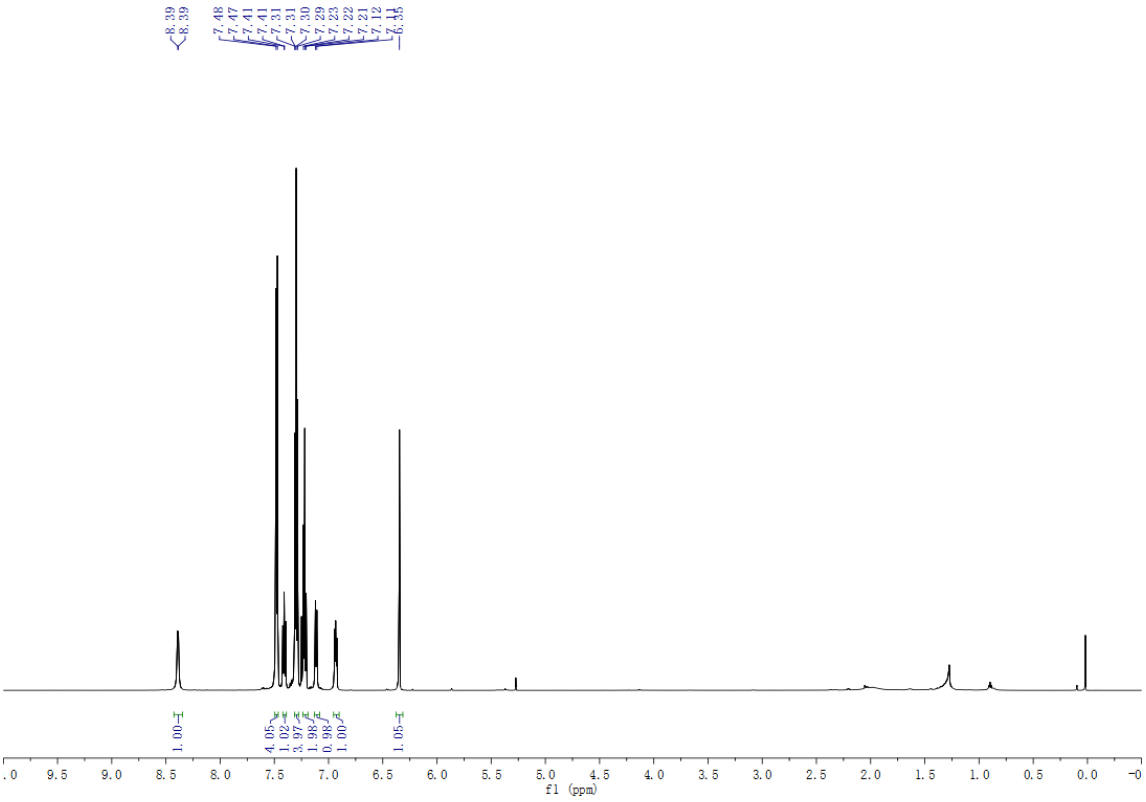
^{13}C NMR ($CDCl_3$, 150 M Hz)



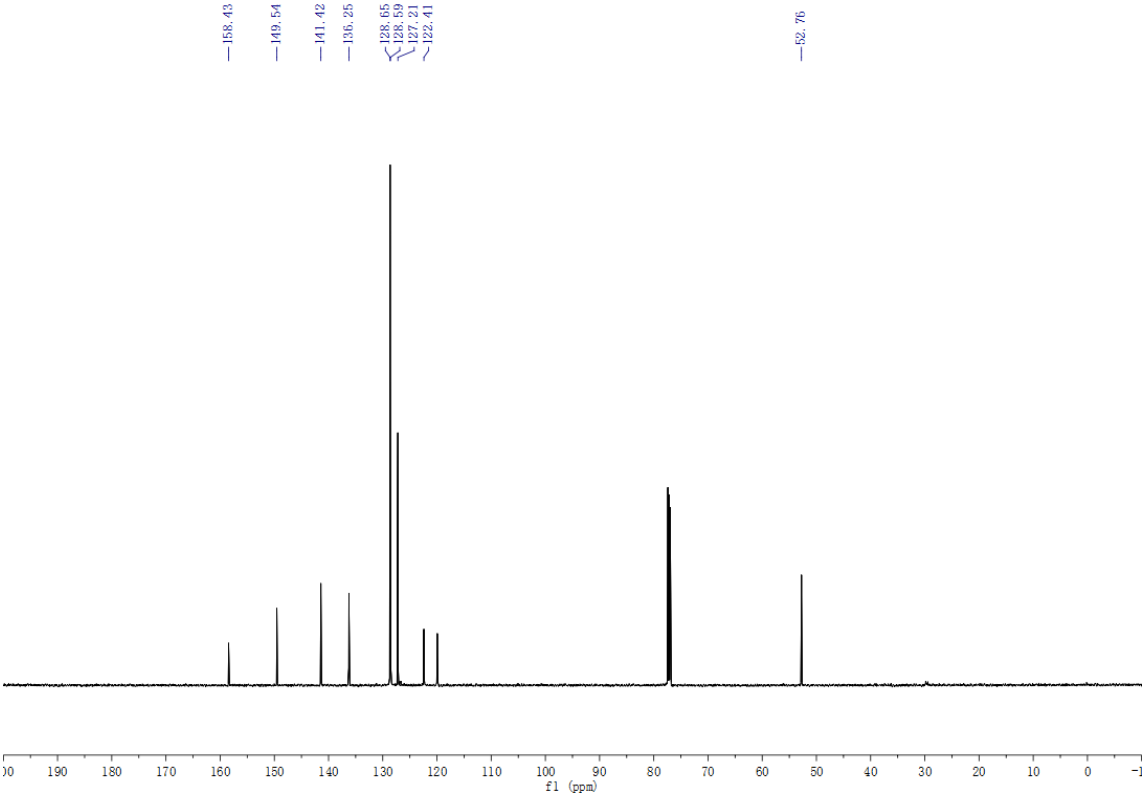


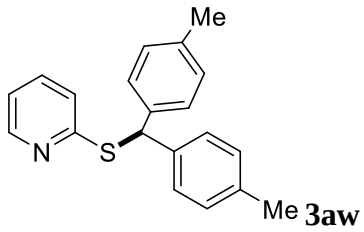
3av

^{1}H NMR ($CDCl_3$, 600 M Hz)



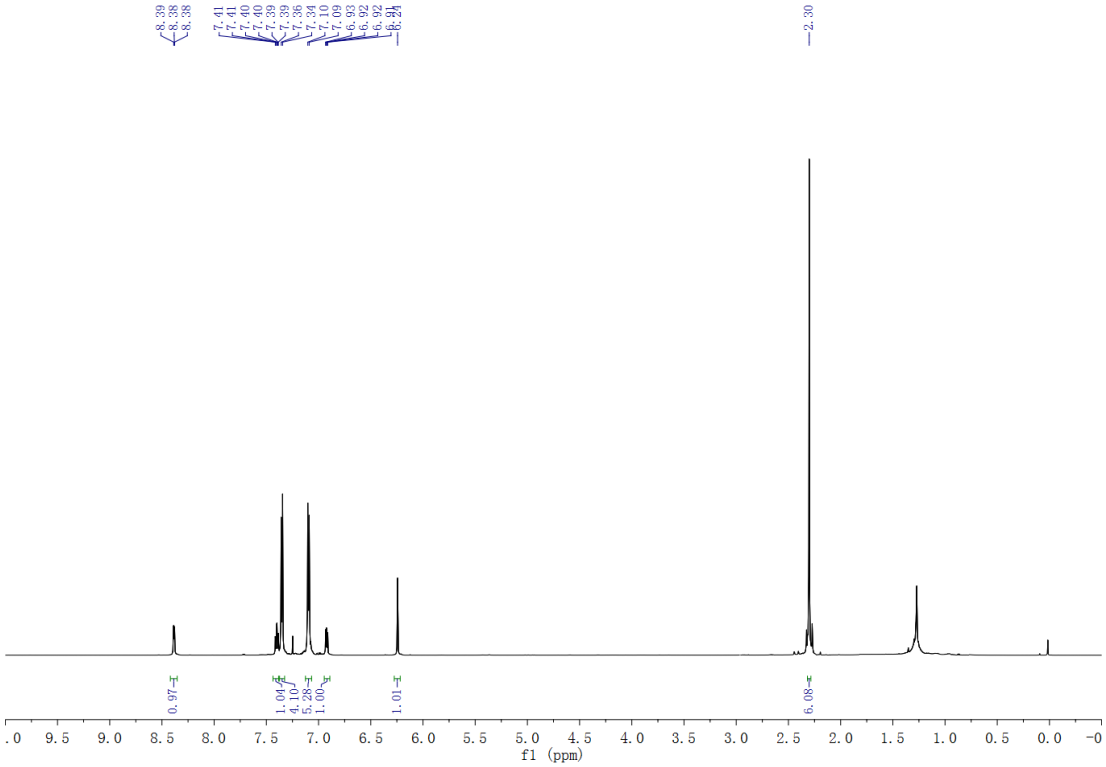
^{13}C NMR ($CDCl_3$, 150 M Hz)



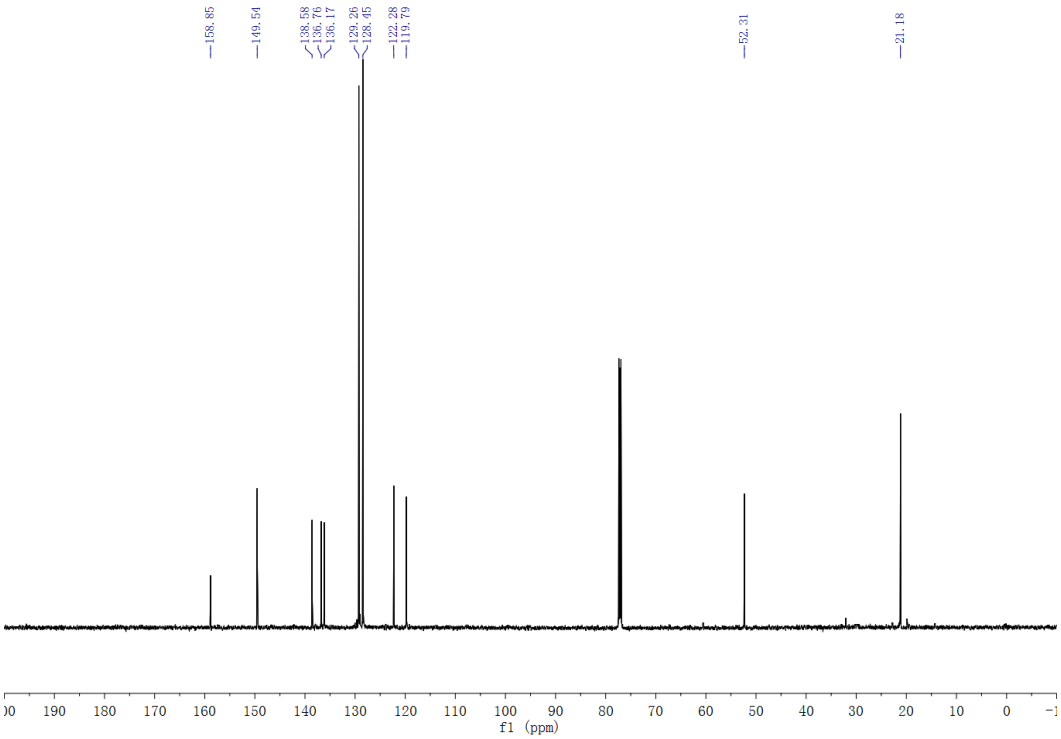


3aw

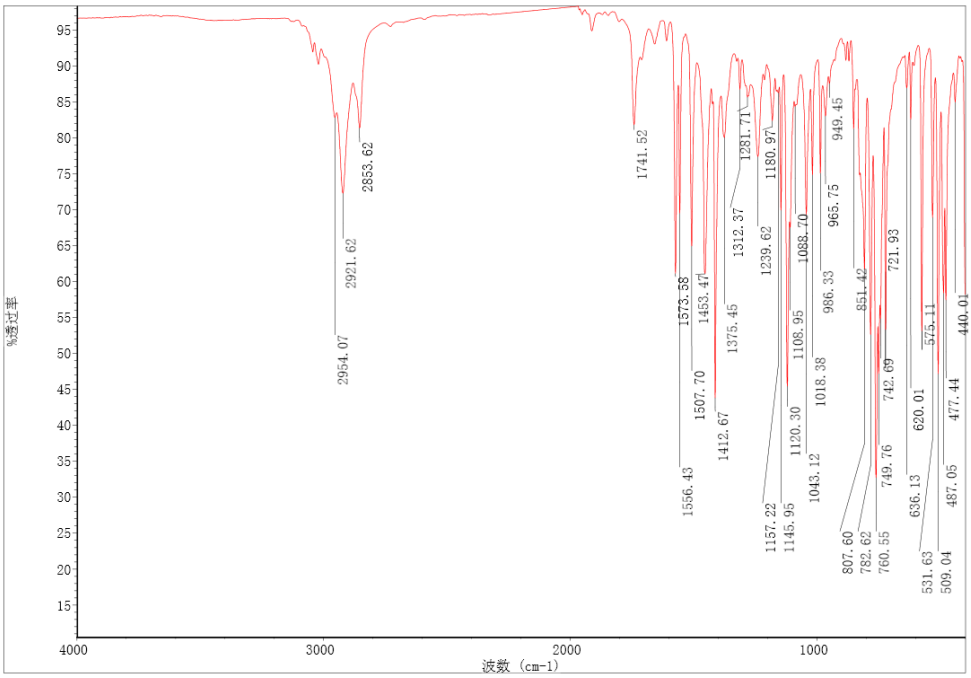
^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)



IR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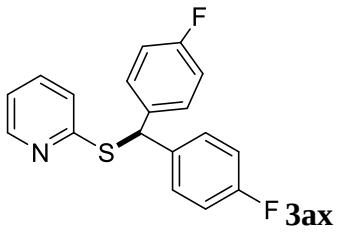
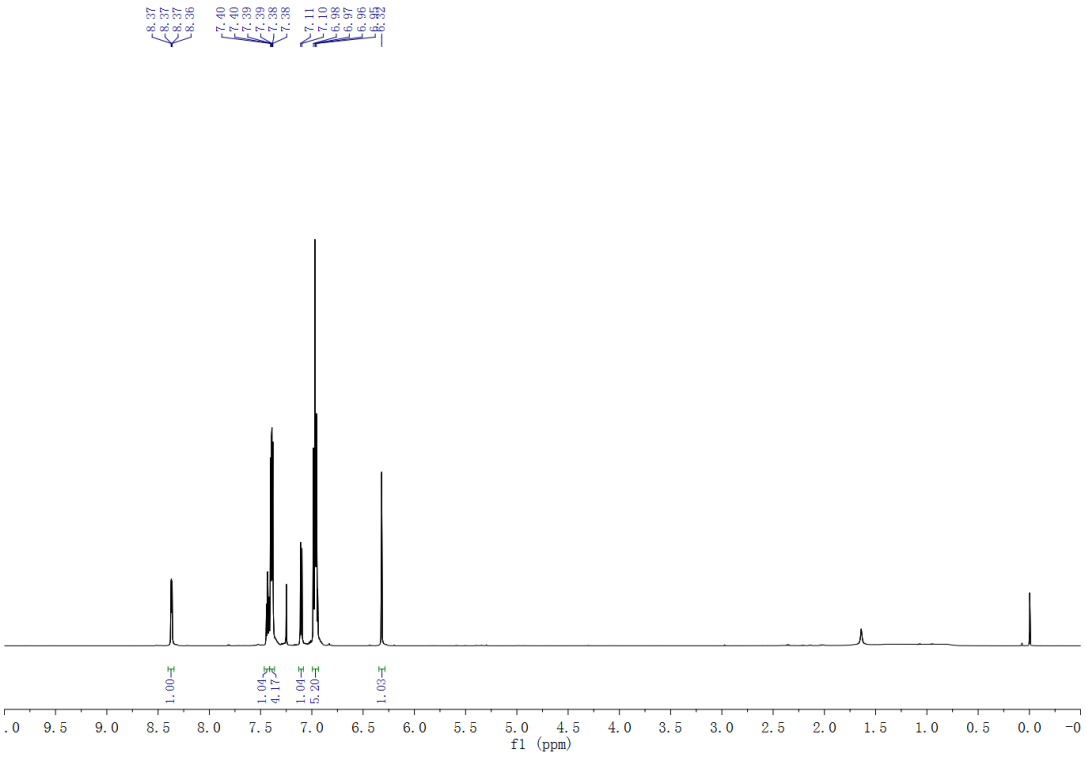
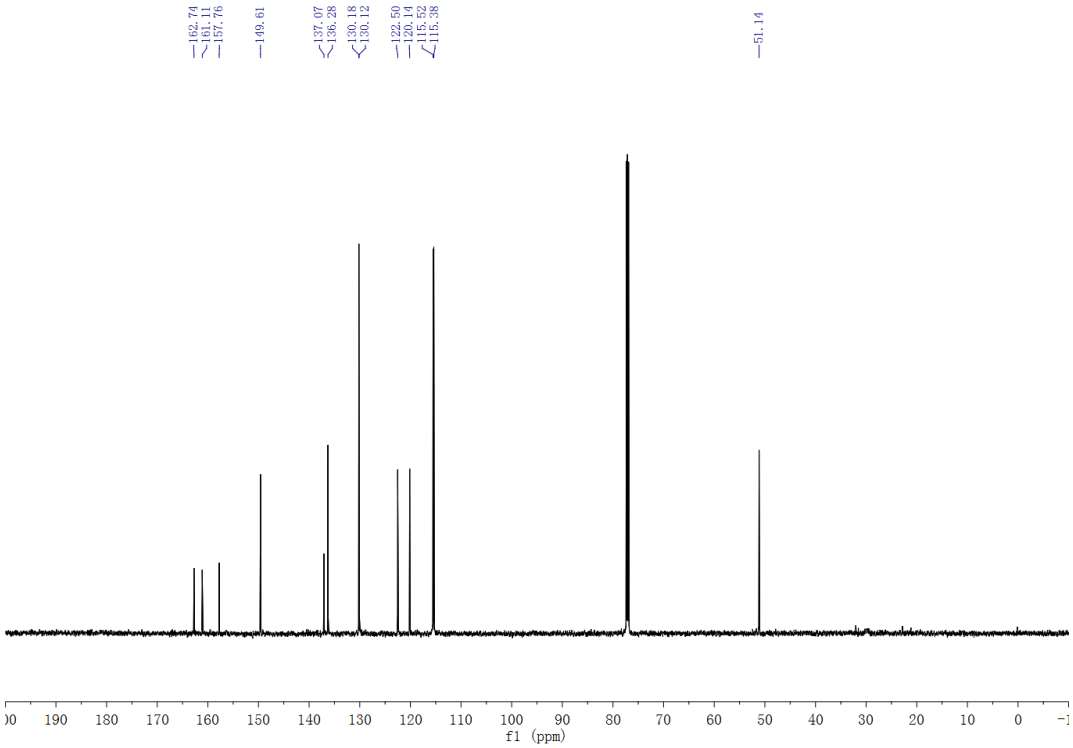


3ax

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)



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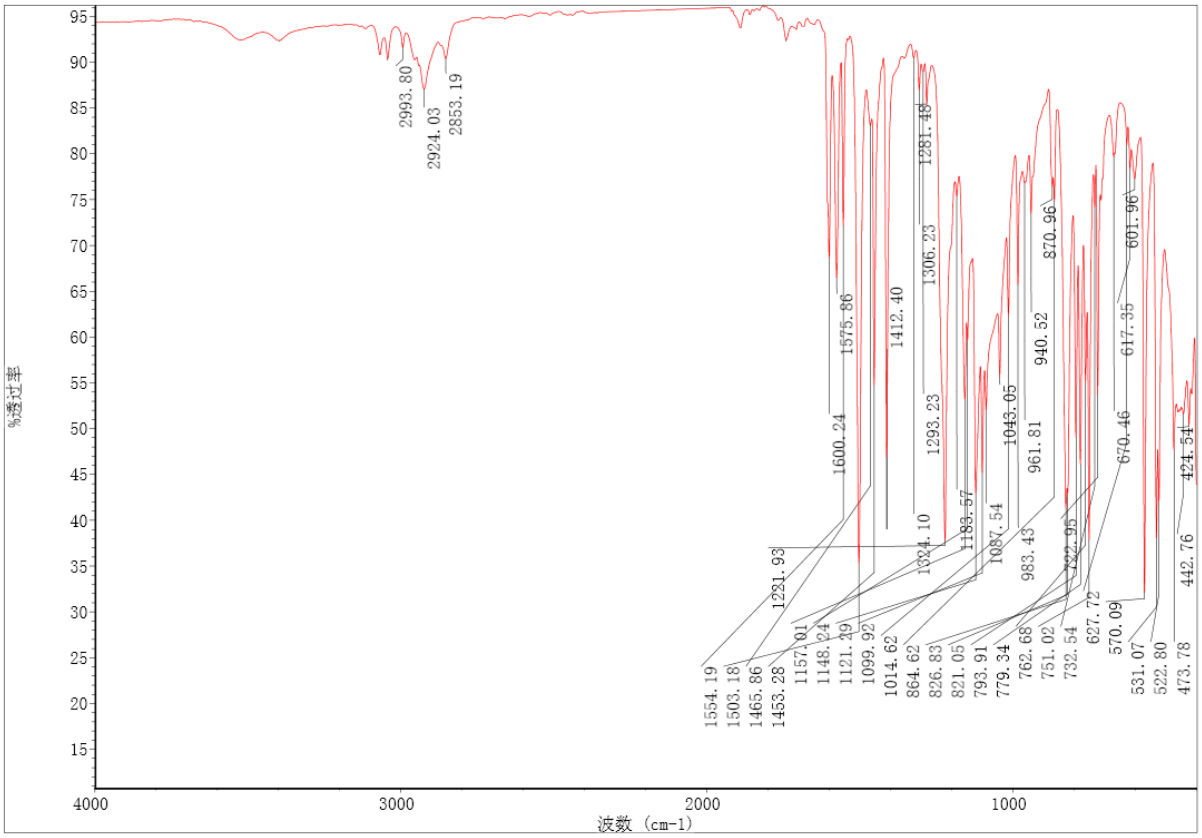
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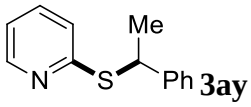
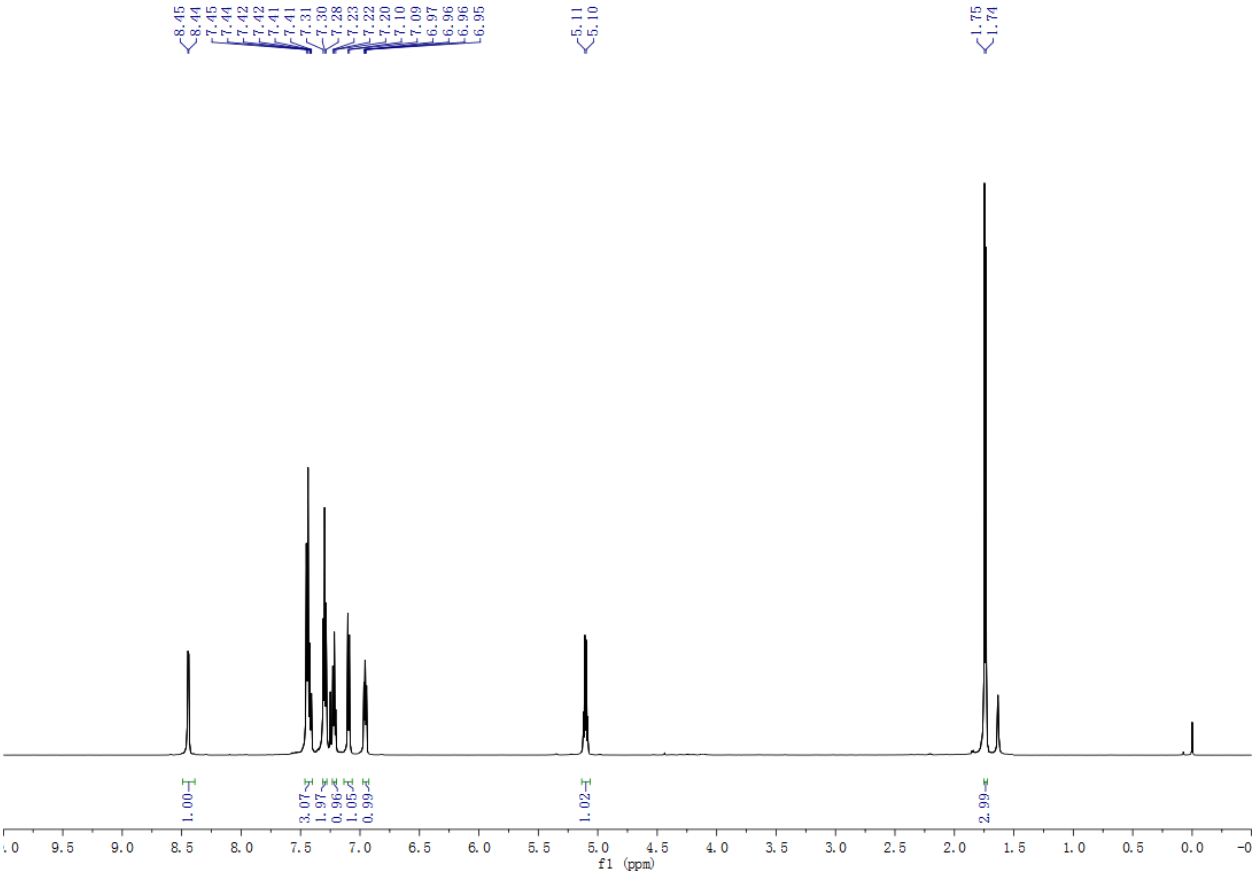
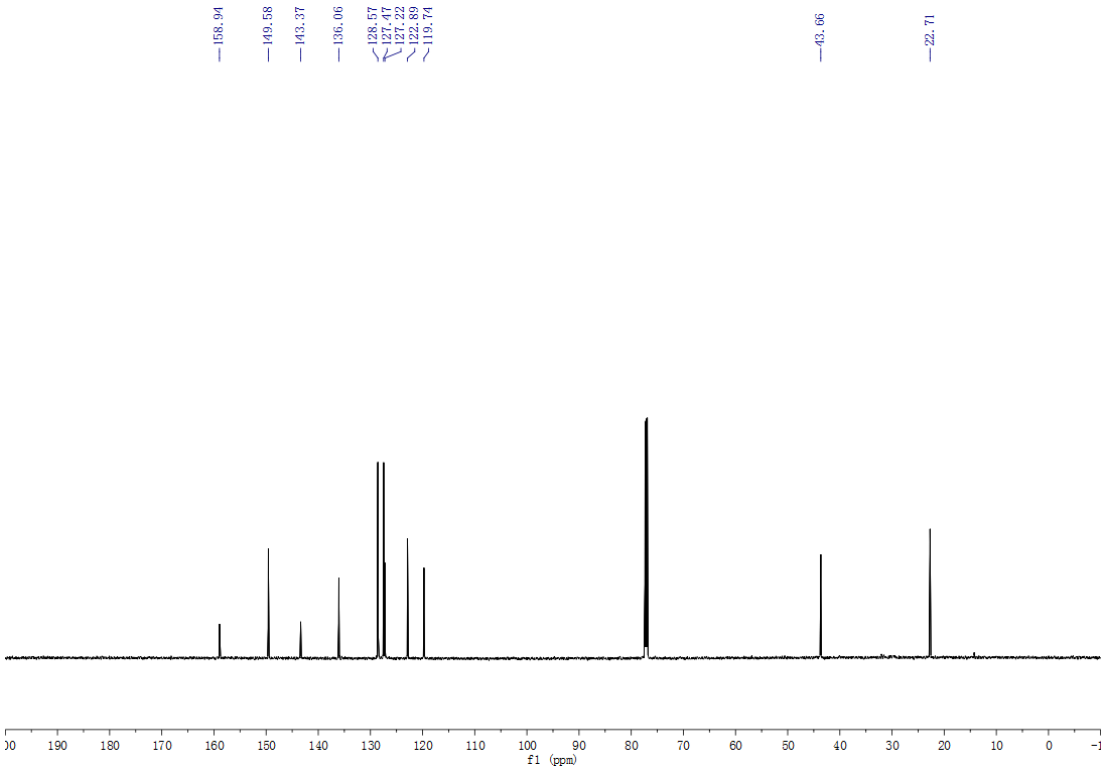


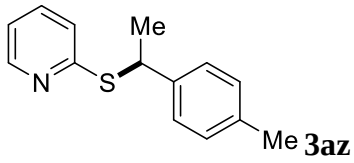
3ay

^{1}H NMR ($CDCl_3$, 600 M Hz)



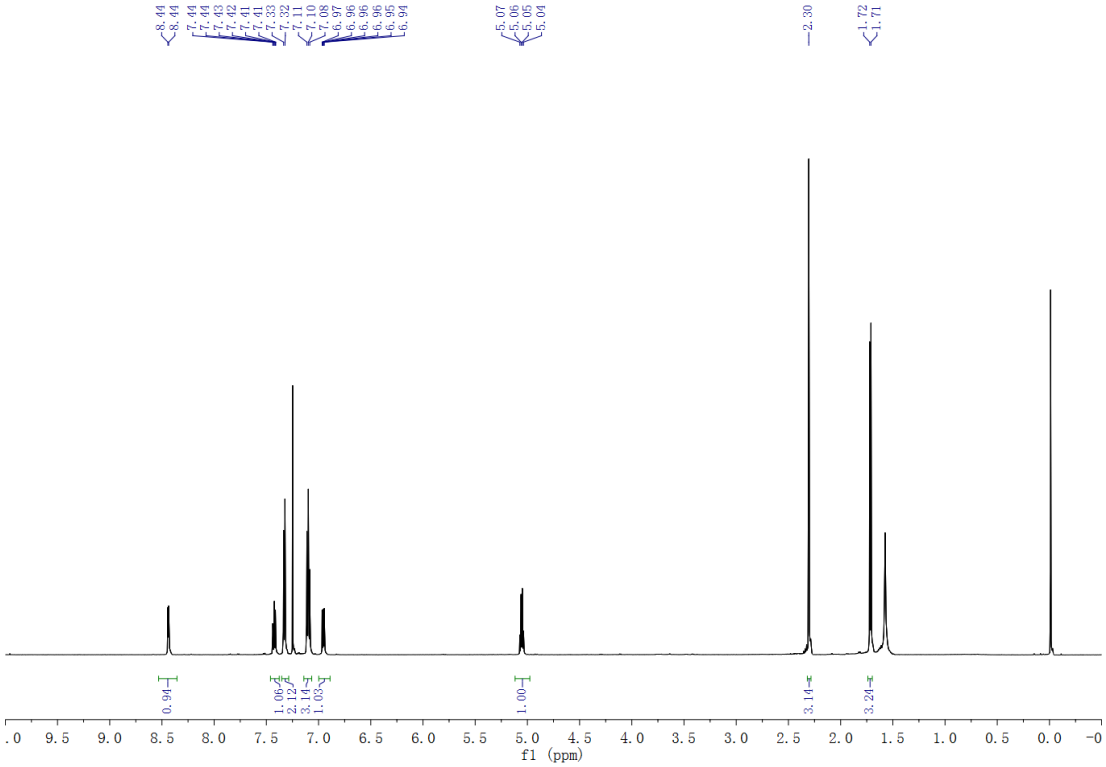
^{13}C NMR ($CDCl_3$, 150 M Hz)



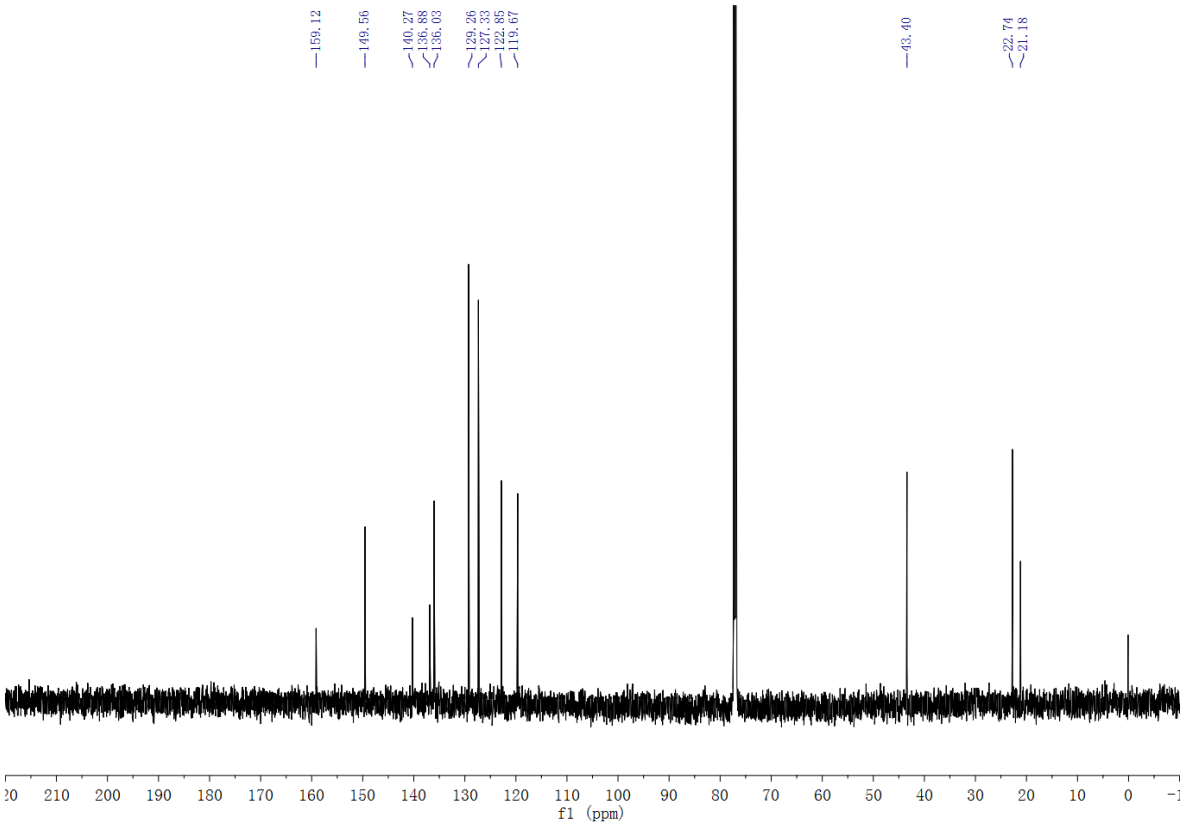


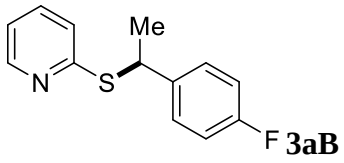
3az

^{1}H NMR ($CDCl_3$, 600 M Hz)



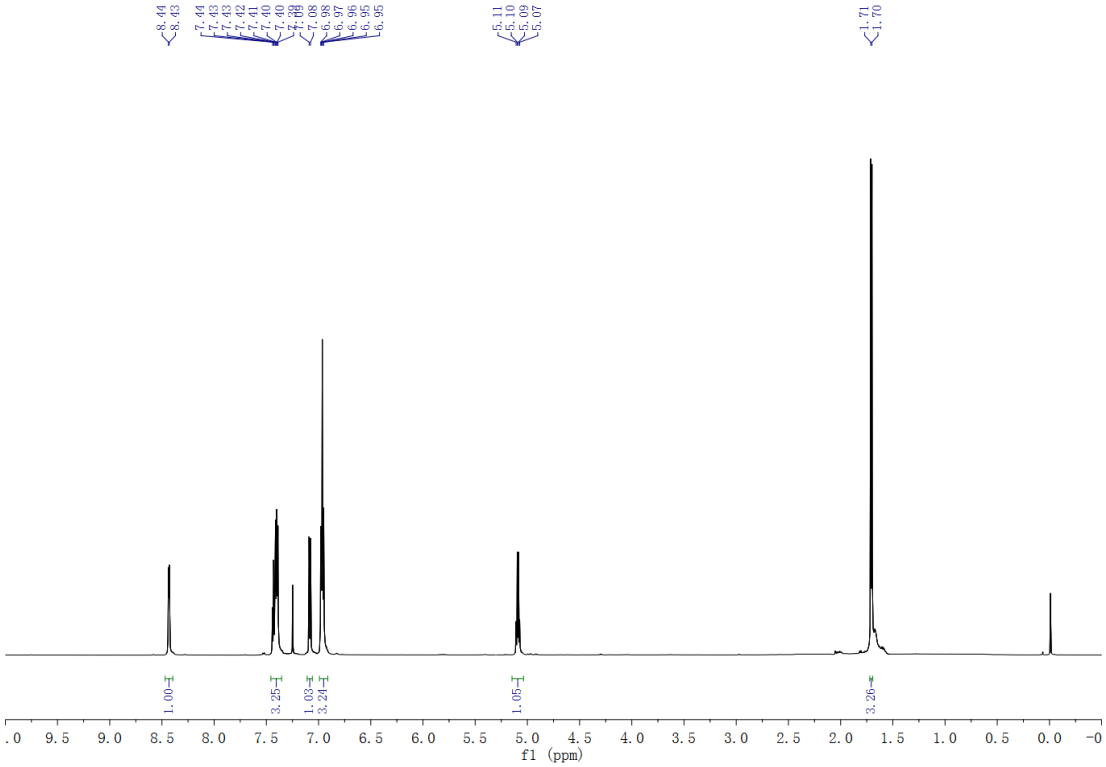
^{13}C NMR ($CDCl_3$, 150 M Hz)



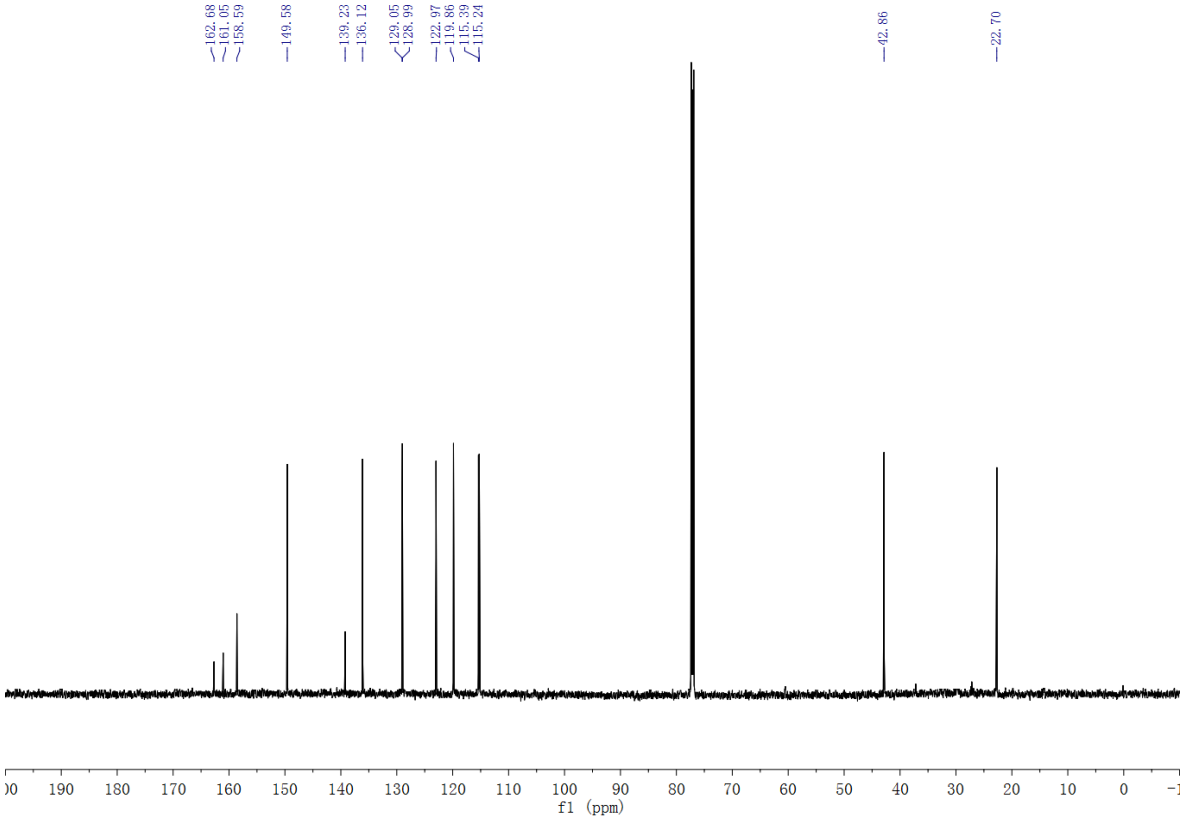


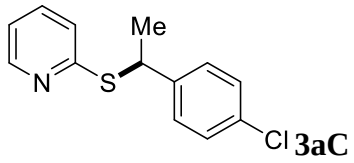
3aB

^{1}H NMR ($CDCl_3$, 600 M Hz)



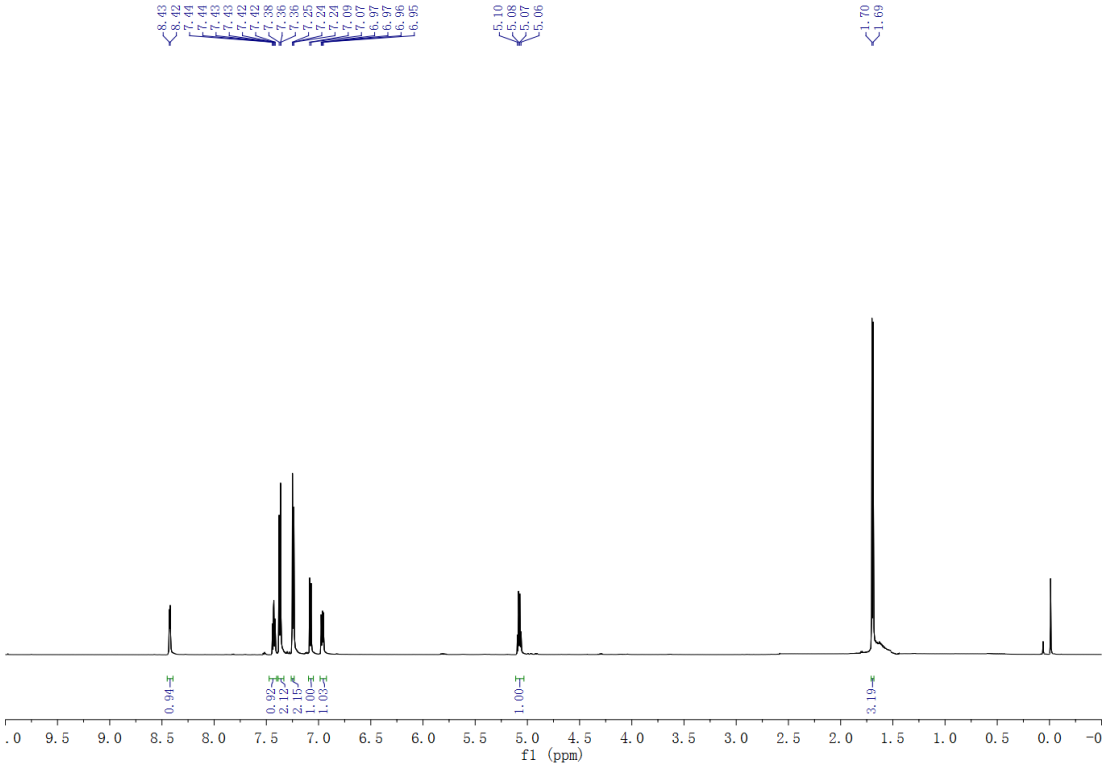
^{13}C NMR ($CDCl_3$, 150 M Hz)



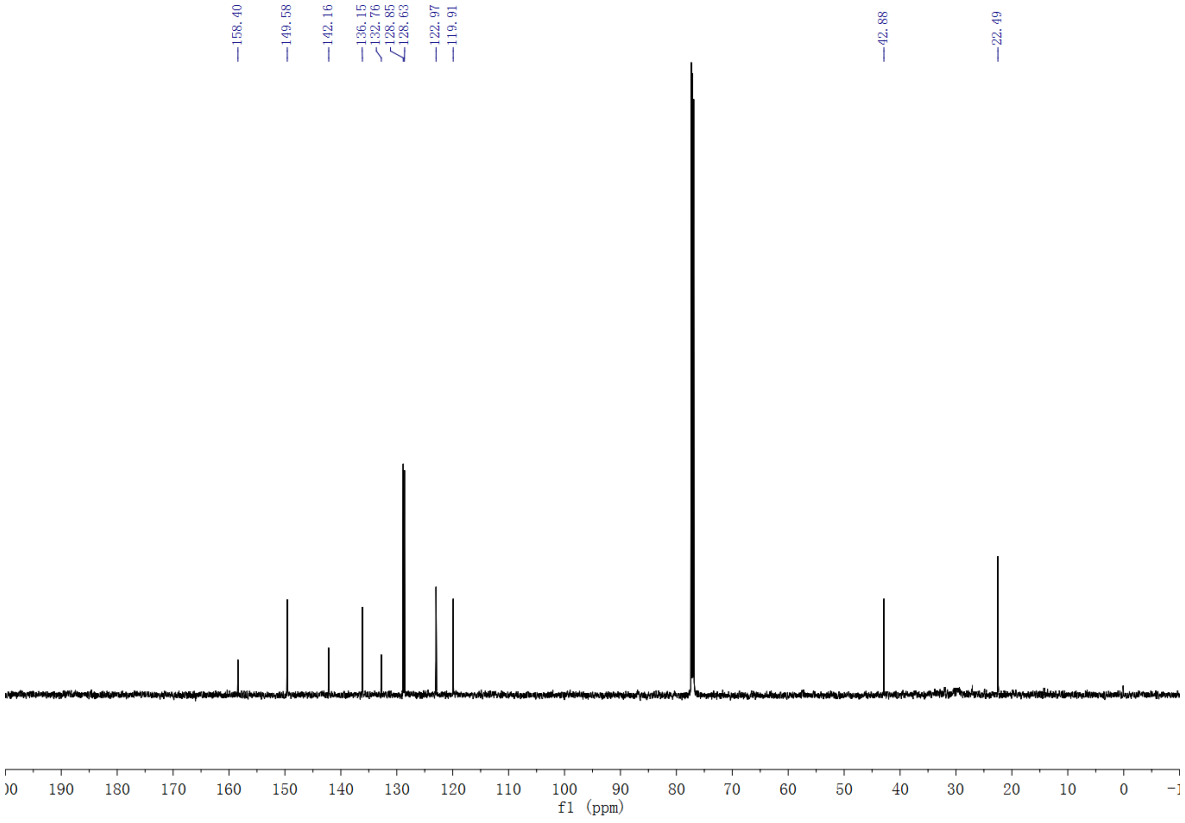


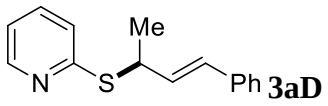
3aC

^{1}H NMR ($CDCl_3$, 600 M Hz)



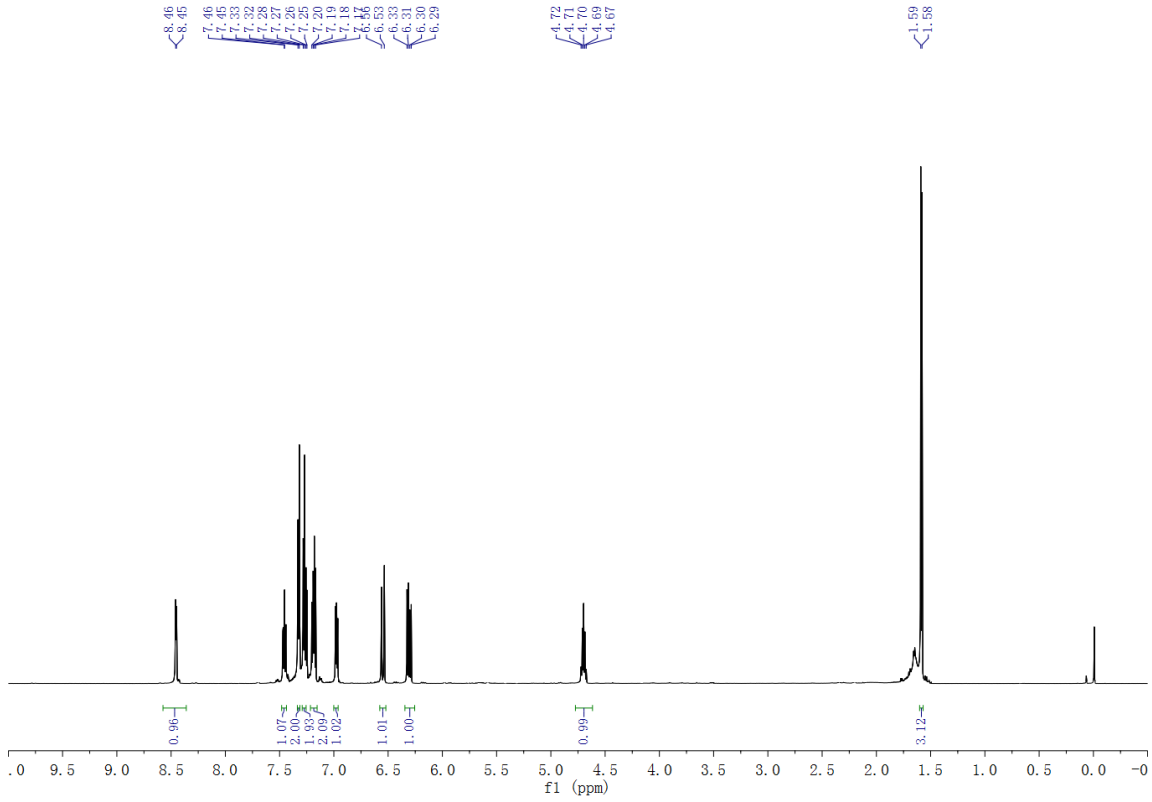
^{13}C NMR ($CDCl_3$, 150 M Hz)



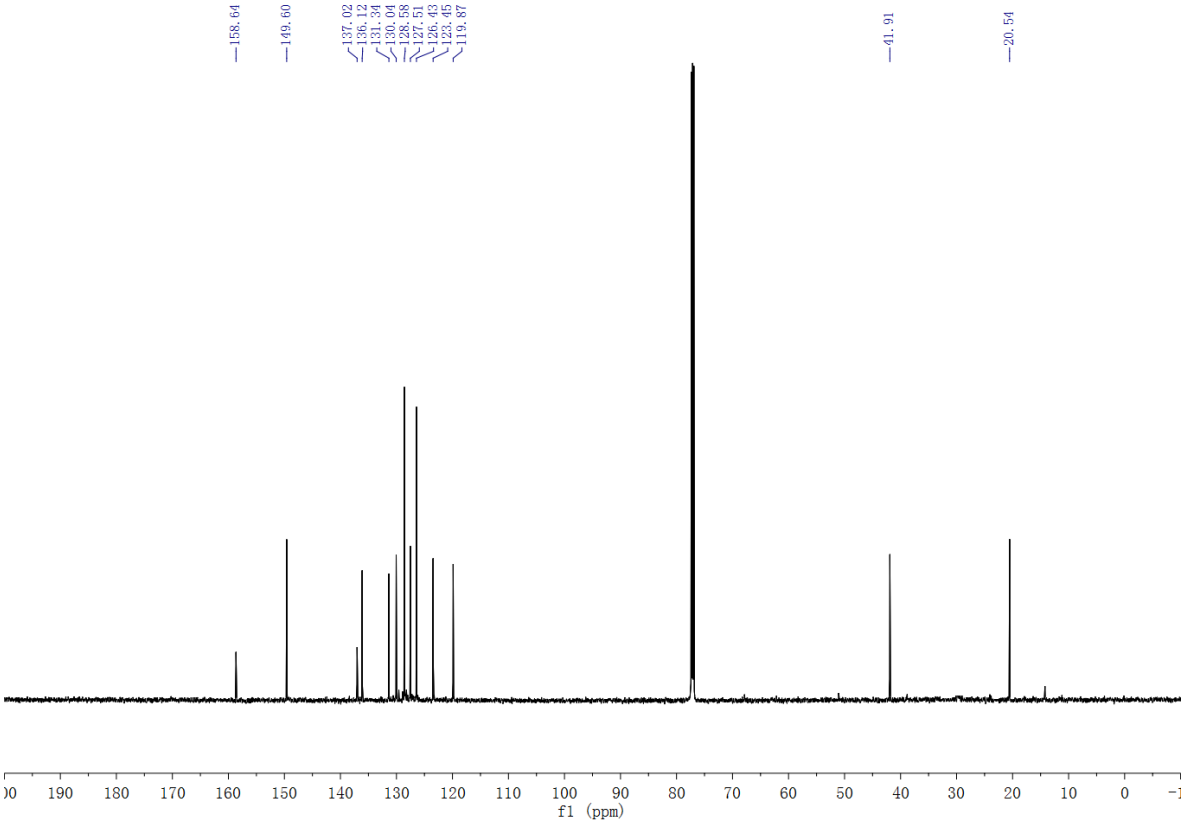


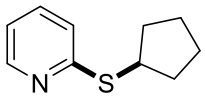
3aD

^{1}H NMR ($CDCl_3$, 600 M Hz)



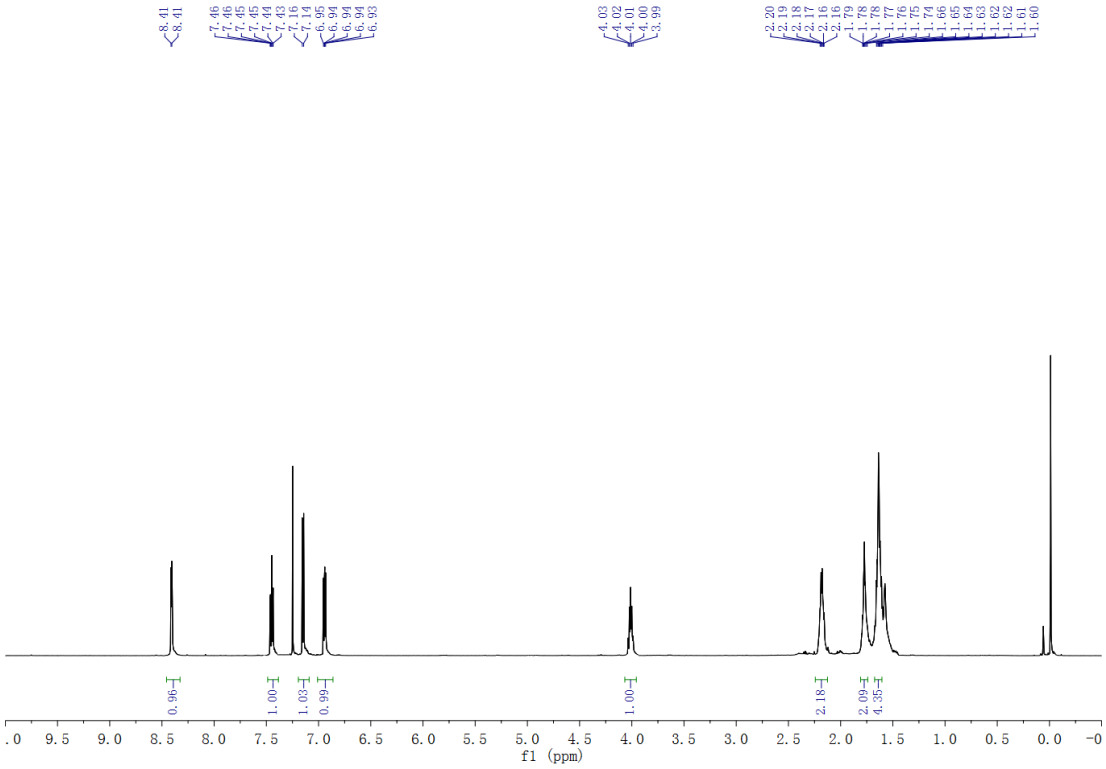
^{13}C NMR ($CDCl_3$, 150 M Hz)



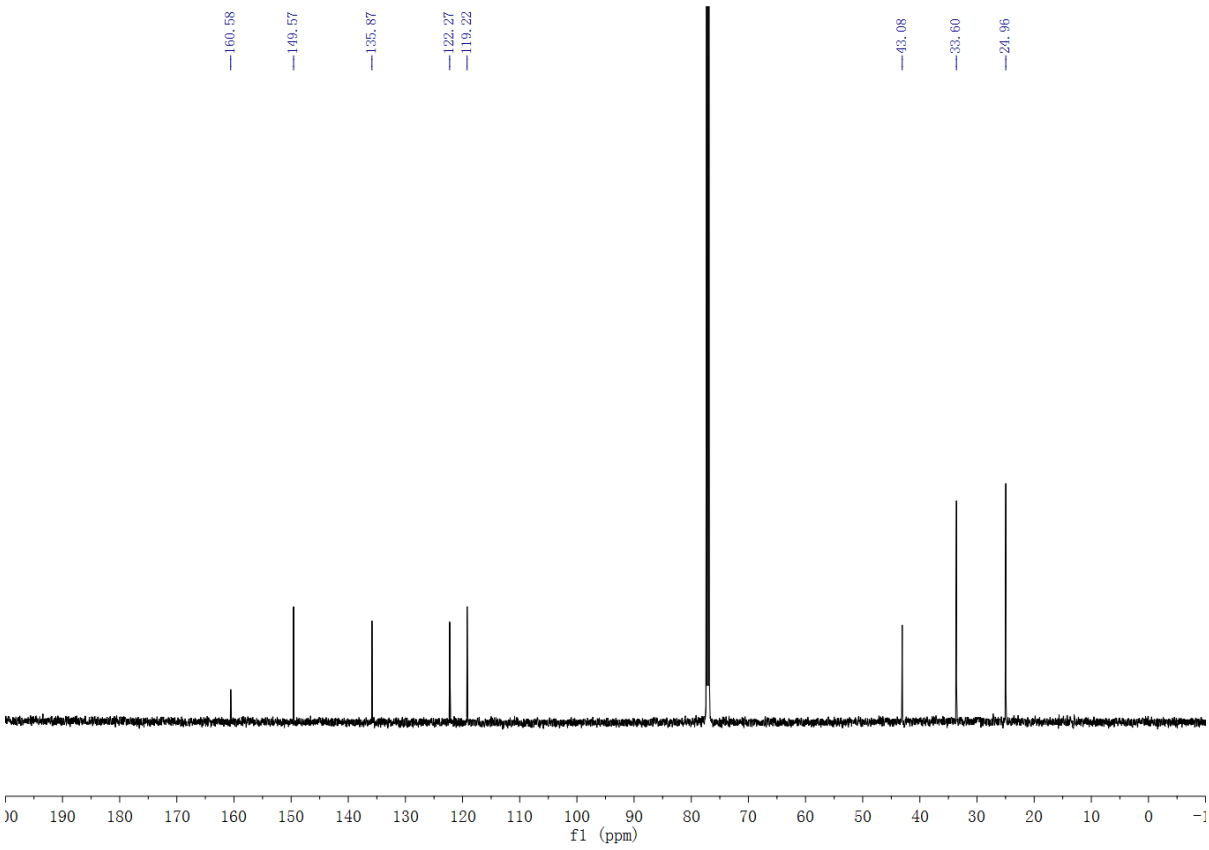


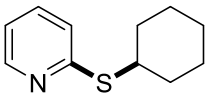
3aE

^{1}H NMR ($CDCl_3$, 600 M Hz)



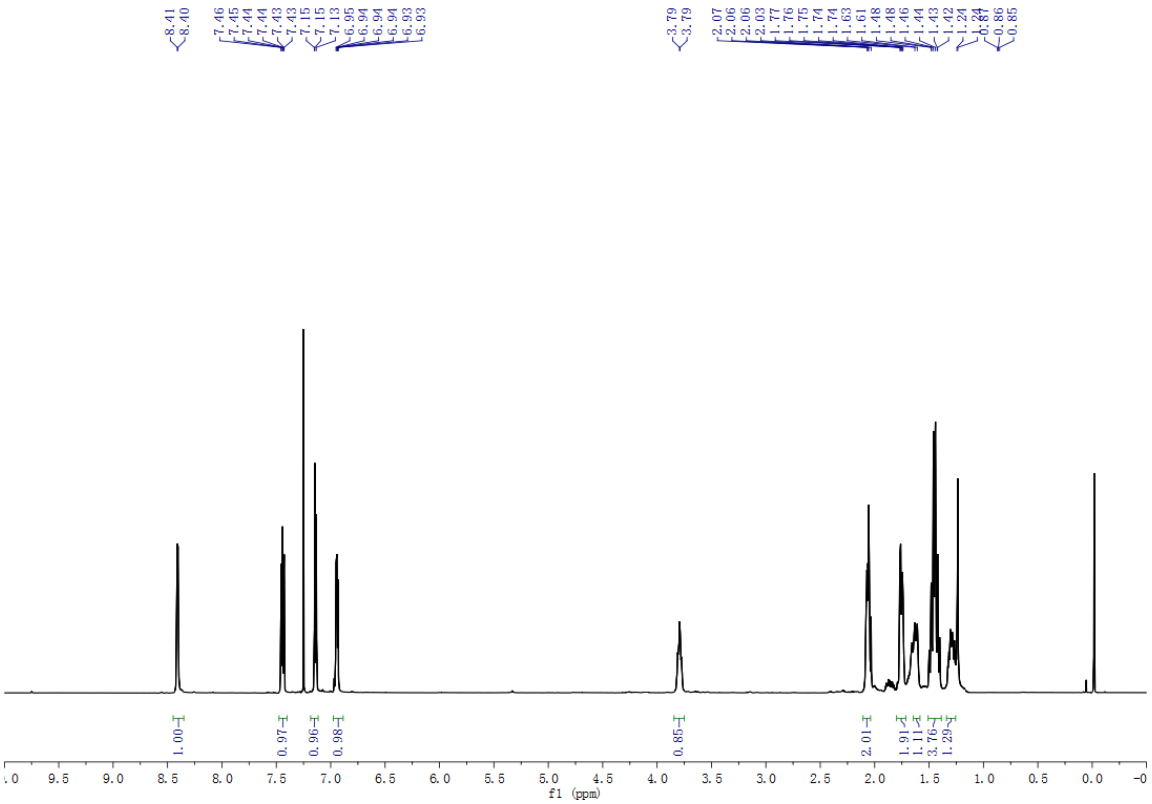
^{13}C NMR ($CDCl_3$, 150 M Hz)



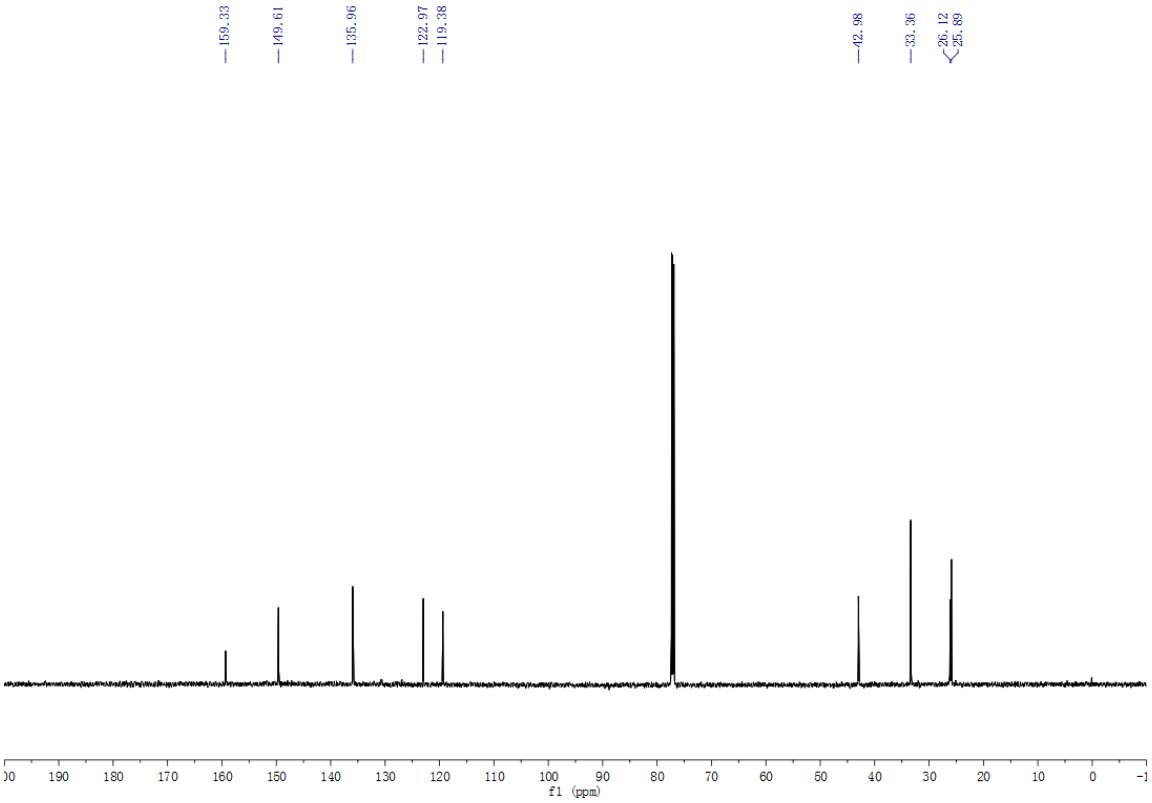


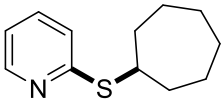
3aF

^{1}H NMR ($CDCl_3$, 600 M Hz)



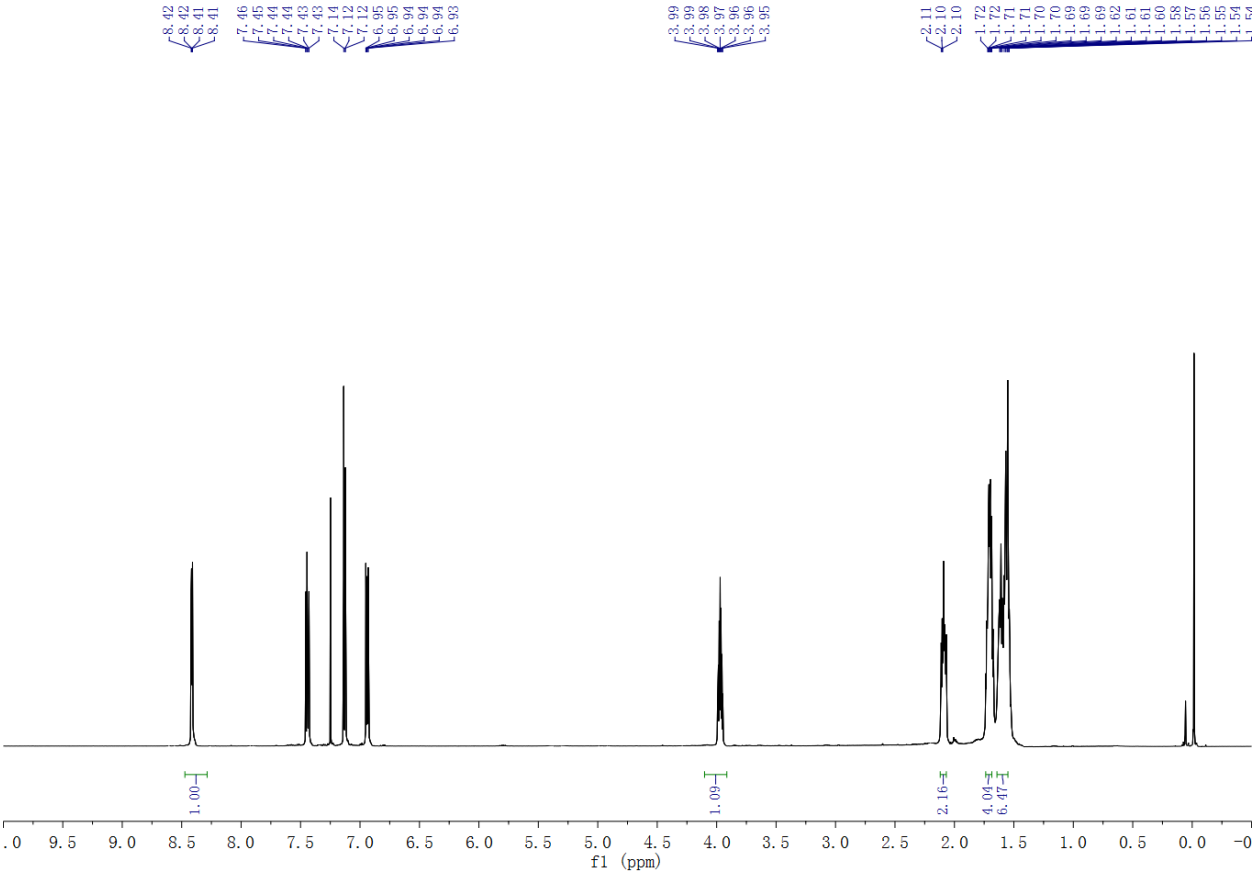
^{13}C NMR ($CDCl_3$, 150 M Hz)



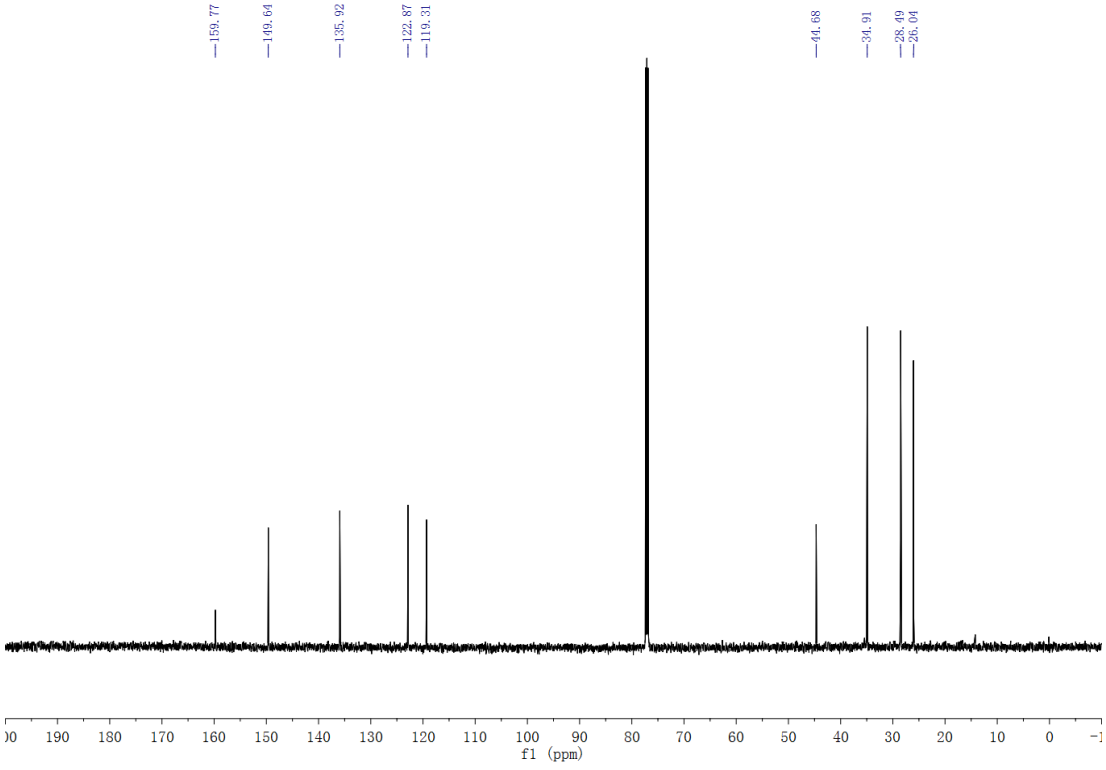


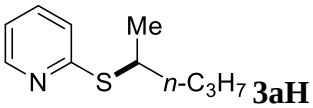
3aG

^{1}H NMR ($CDCl_3$, 600 M Hz)



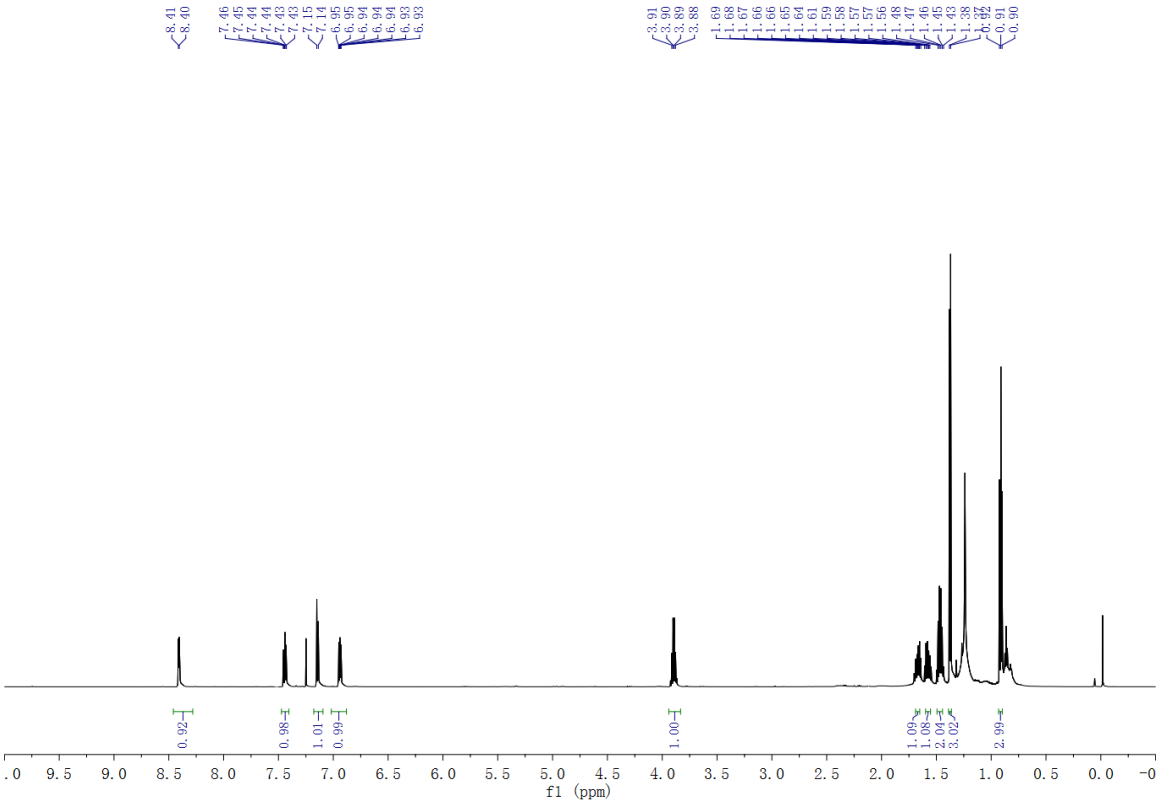
^{13}C NMR ($CDCl_3$, 150 M Hz)



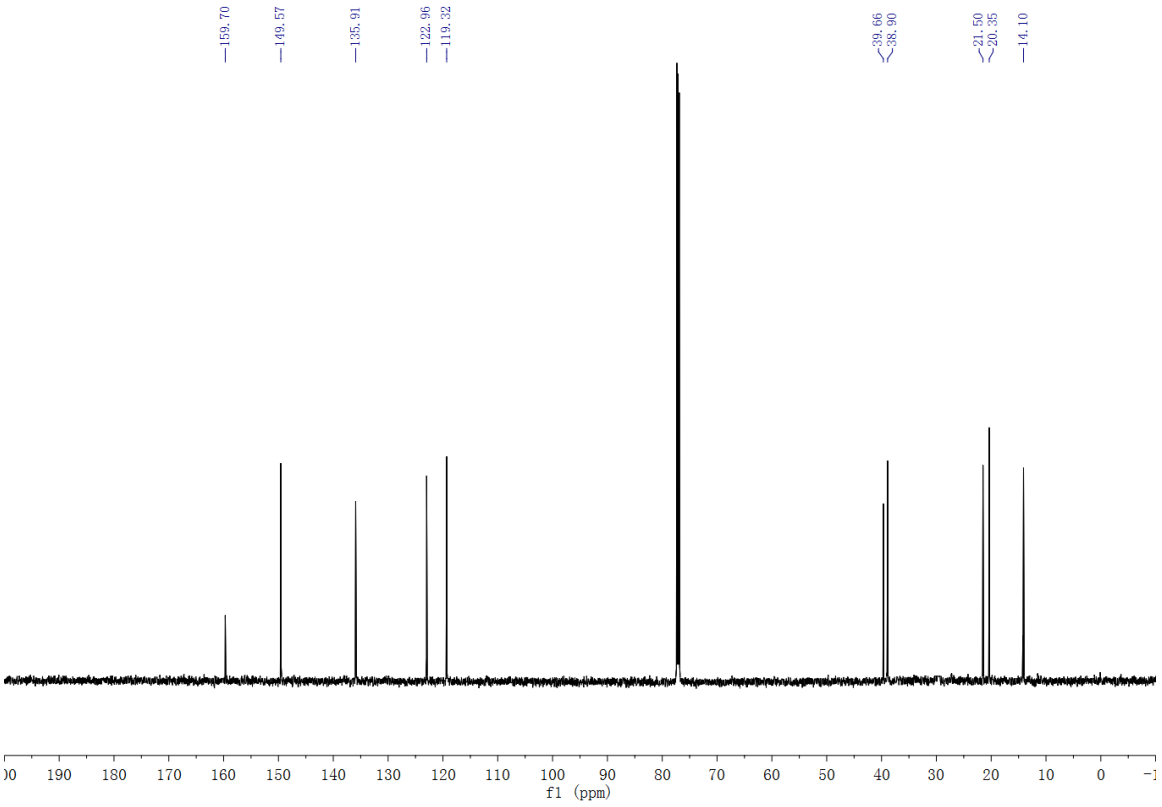


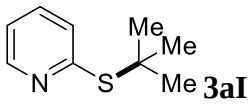
3aH

^{1}H NMR ($CDCl_3$, 600 M Hz)



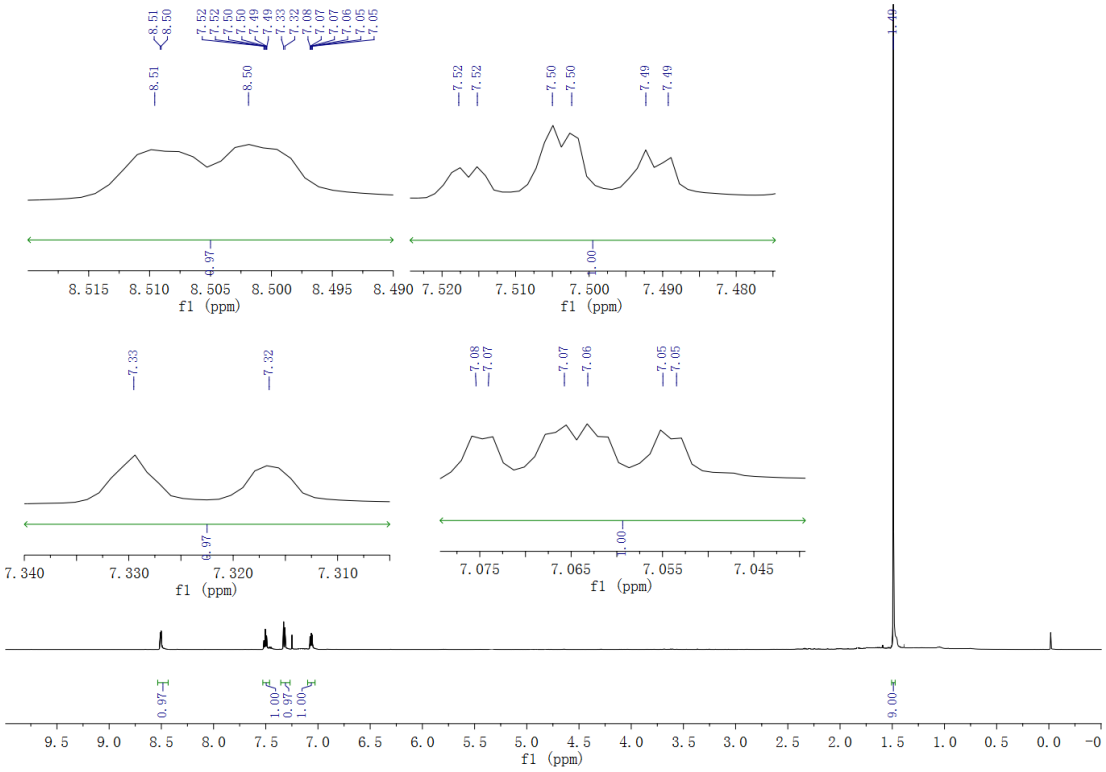
^{13}C NMR ($CDCl_3$, 150 M Hz)



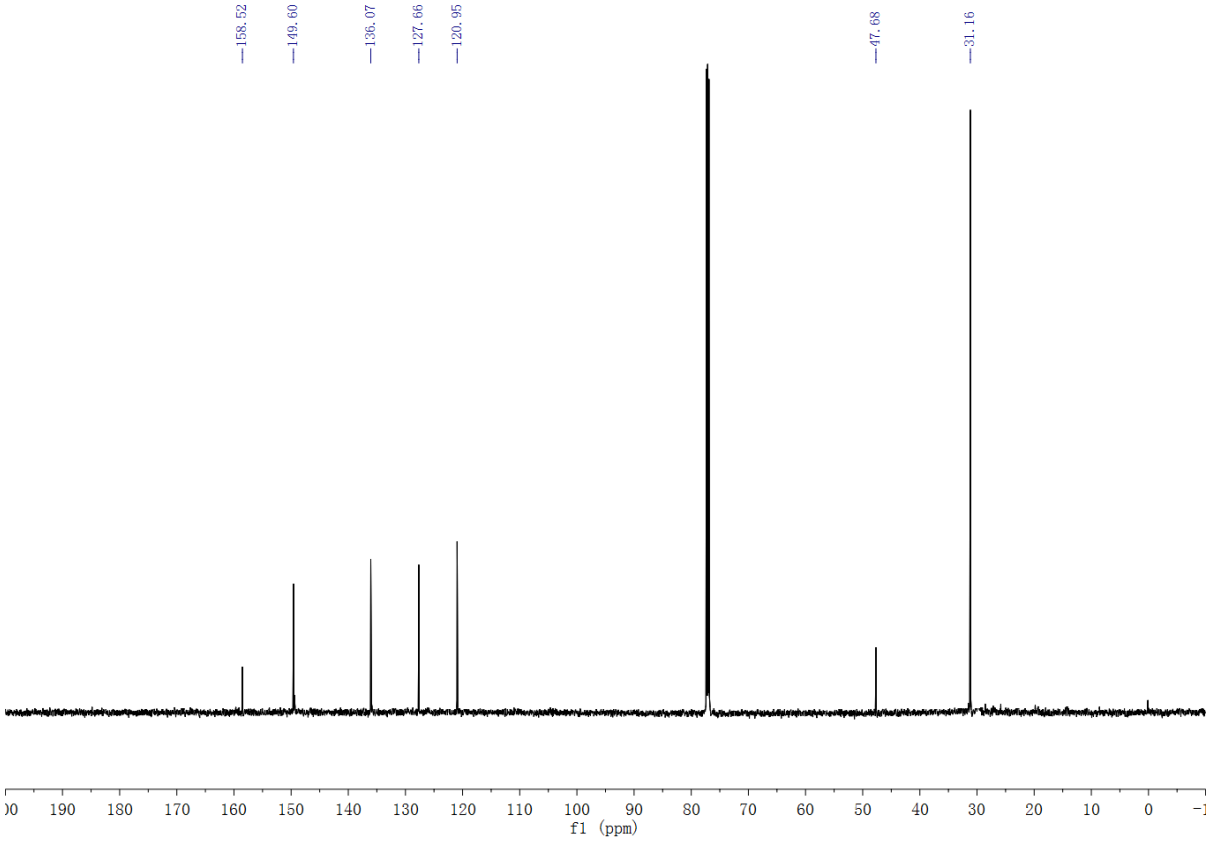


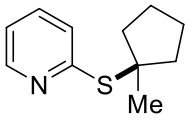
3aI

^{1}H NMR ($CDCl_3$, 600 M Hz)



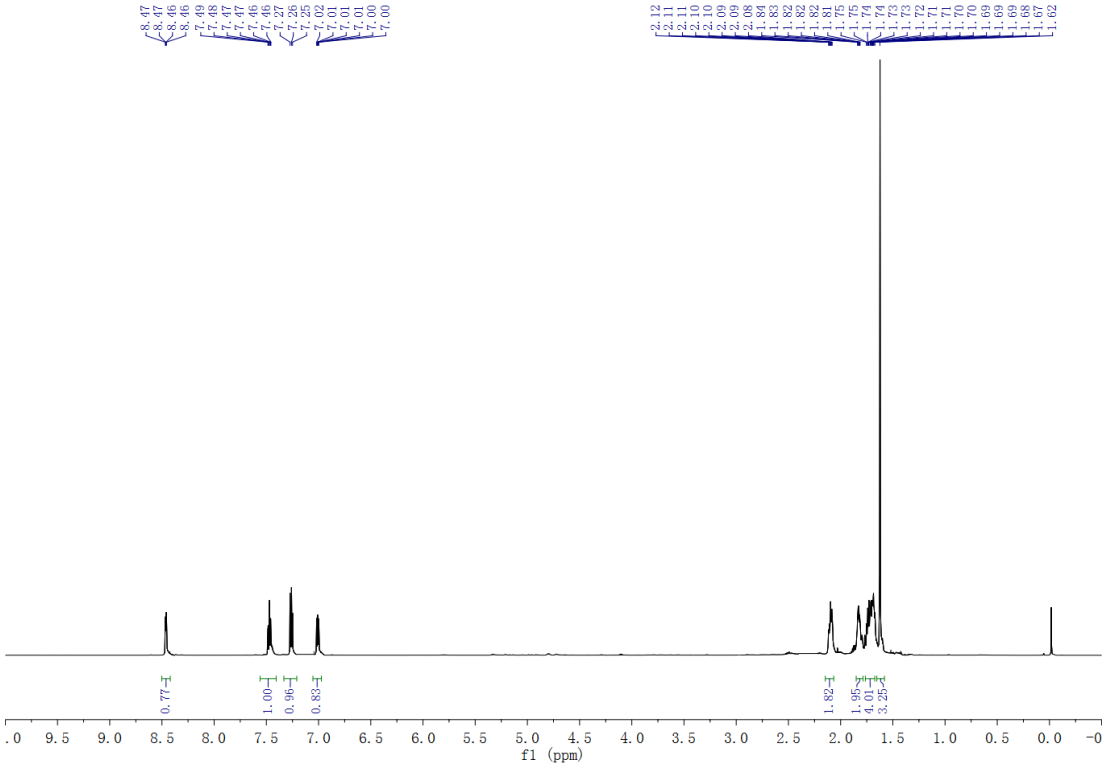
^{13}C NMR ($CDCl_3$, 150 M Hz)



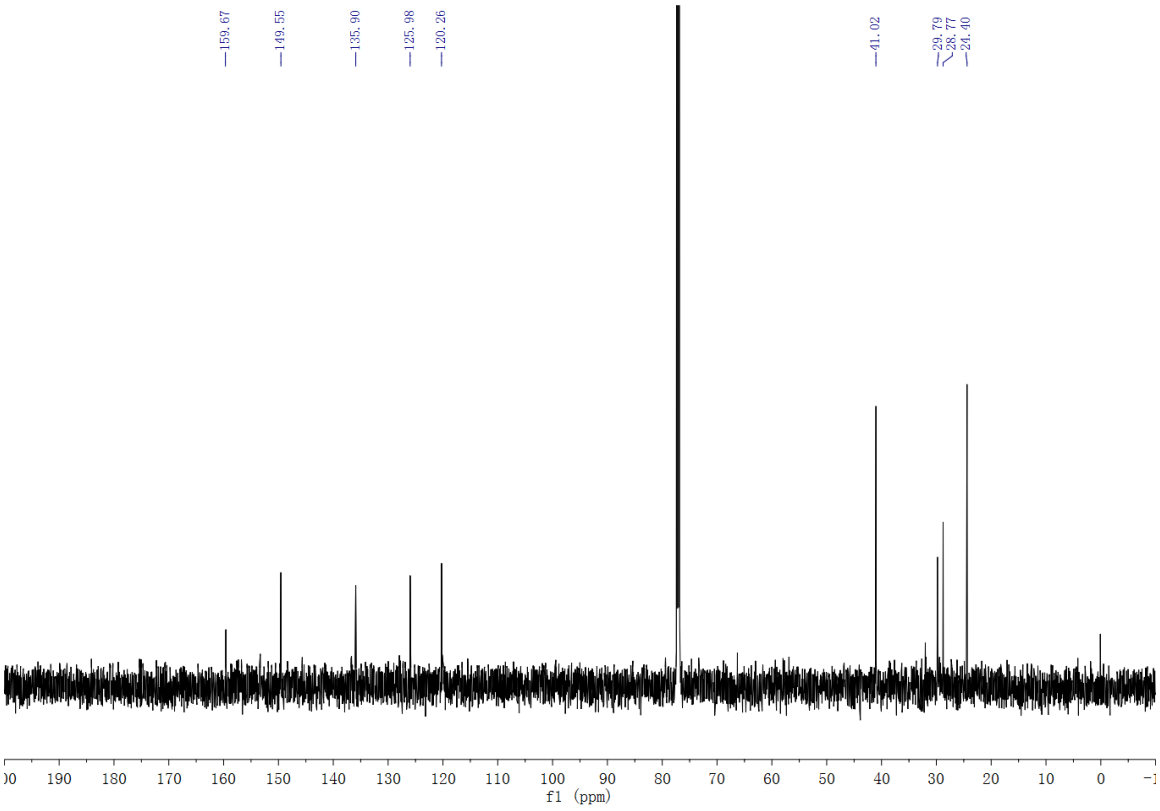


3aJ

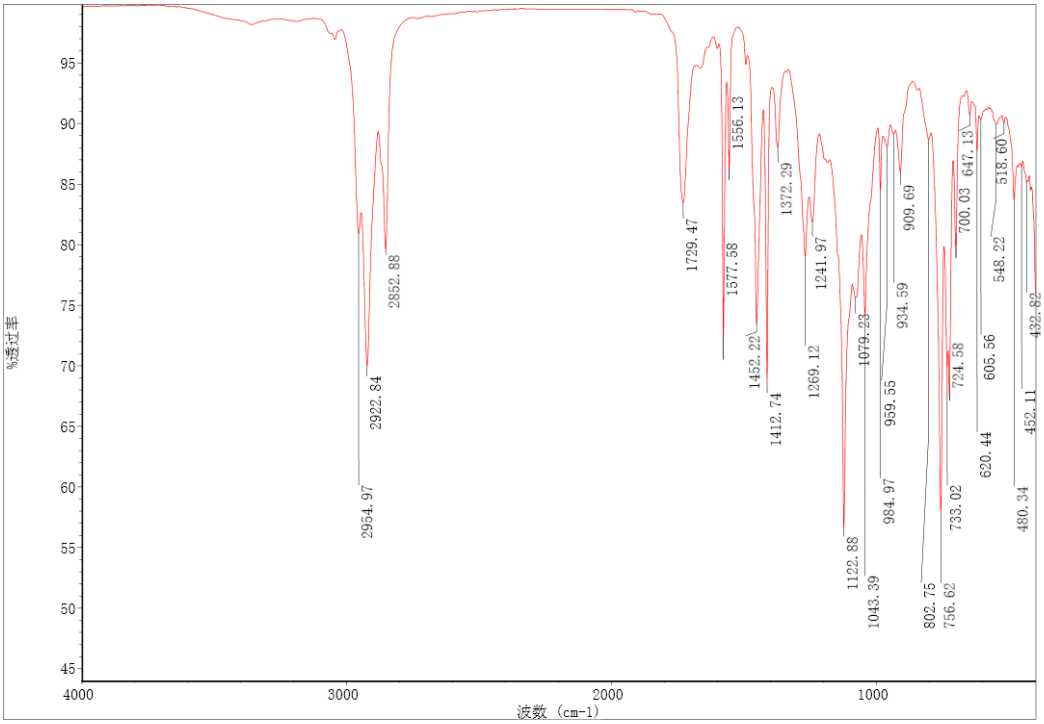
^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)



IR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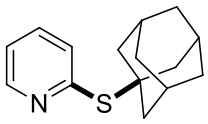
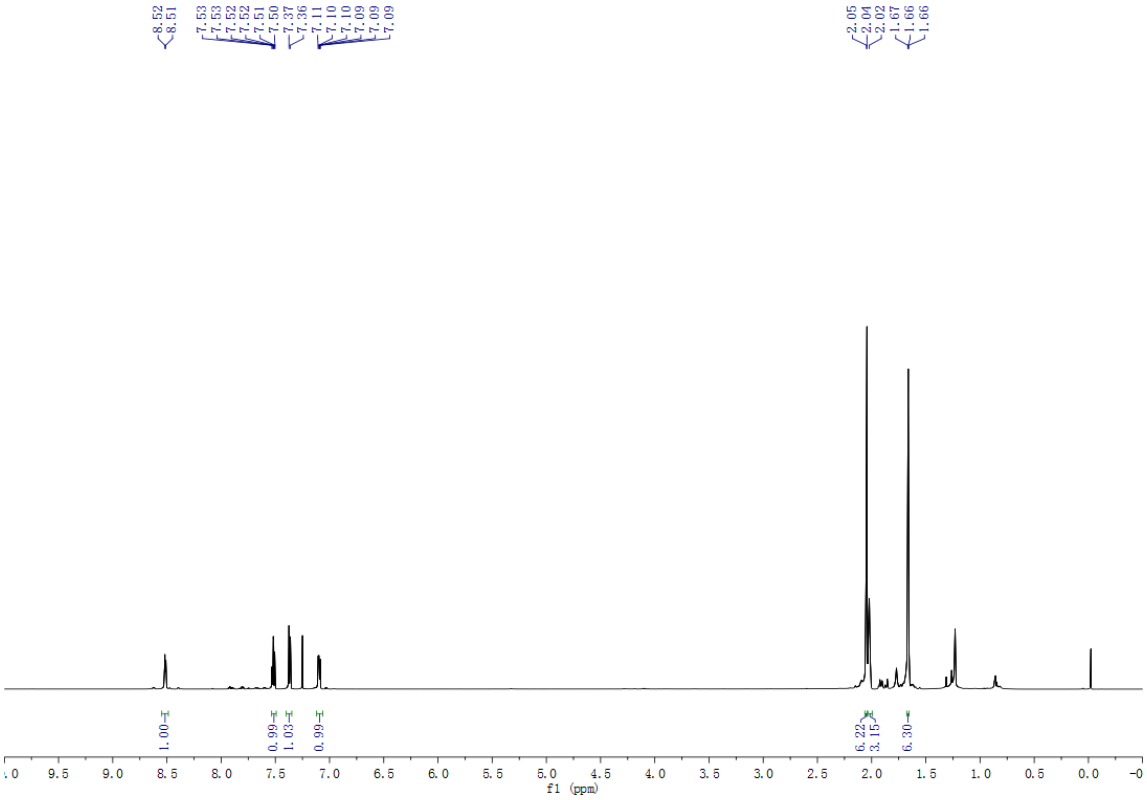
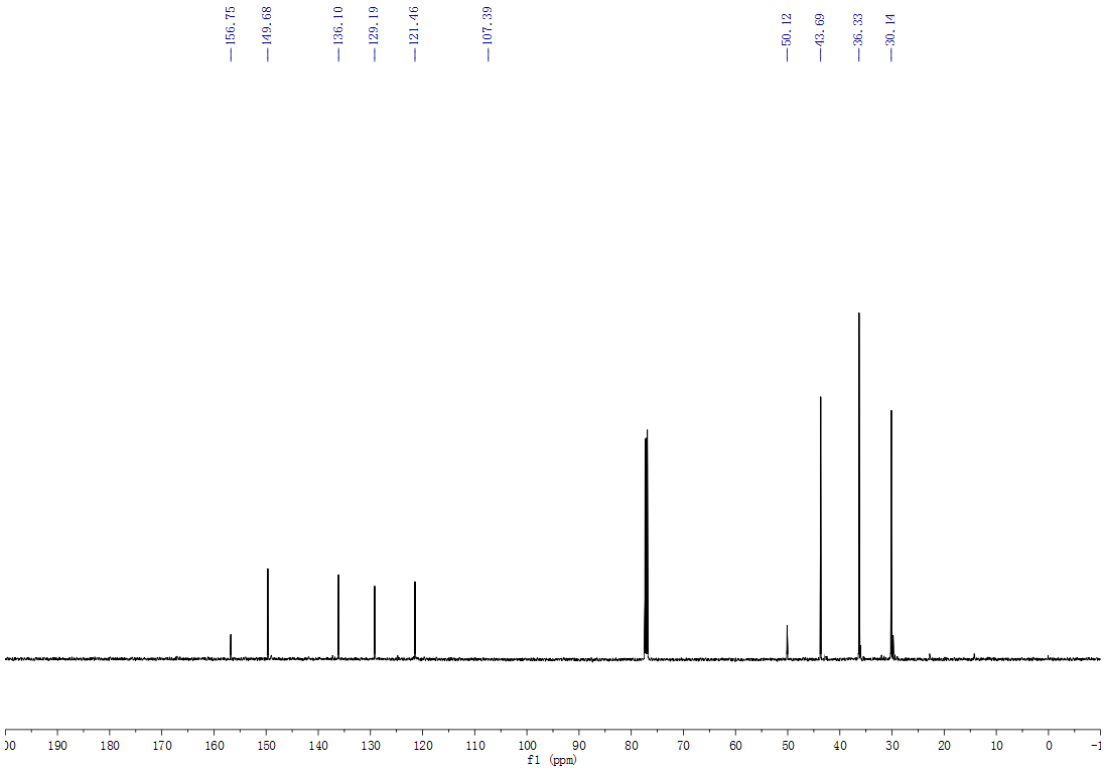


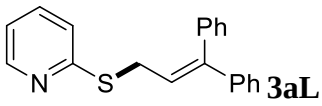
3aK

^{1}H NMR ($CDCl_3$, 600 M Hz)



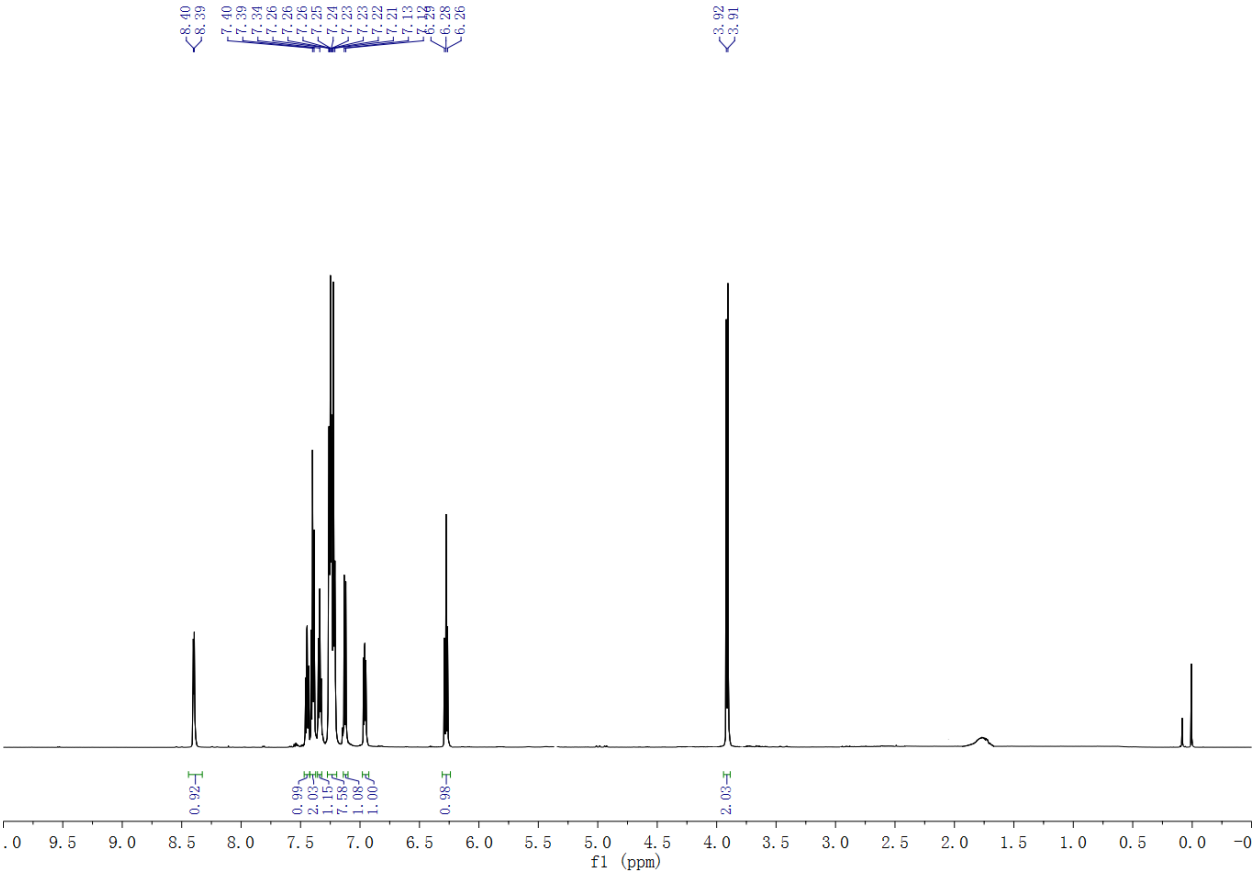
^{13}C NMR ($CDCl_3$, 150 M Hz)



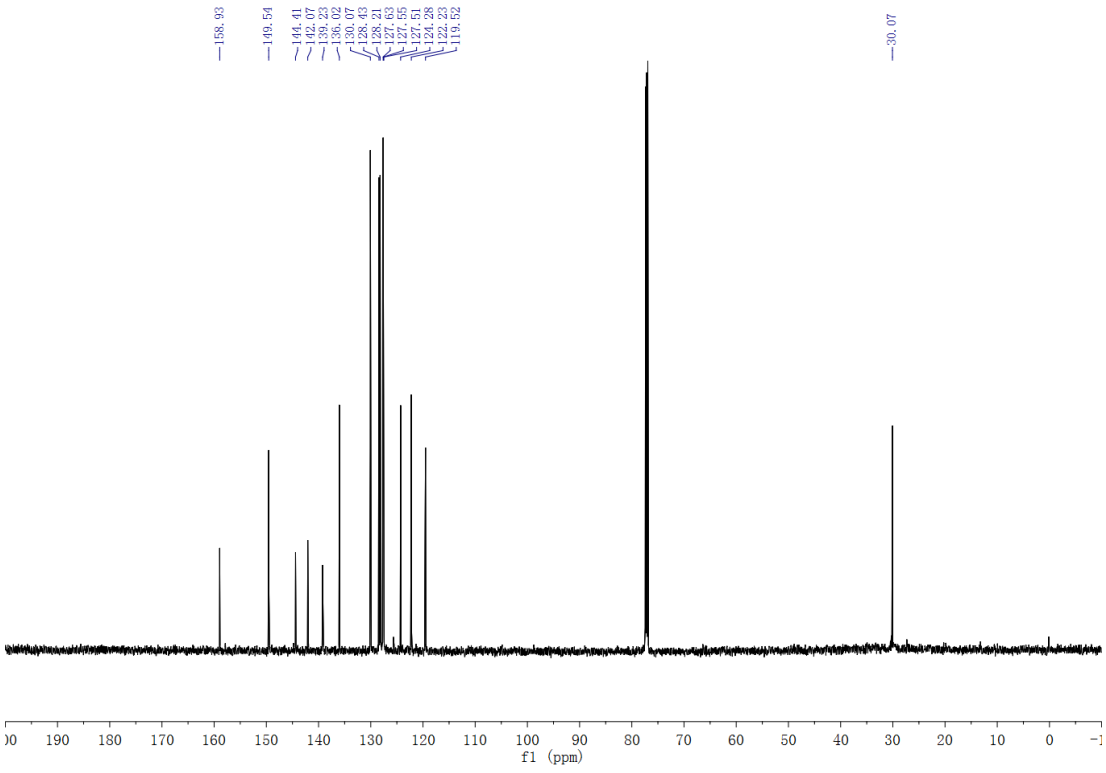


3aL

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)



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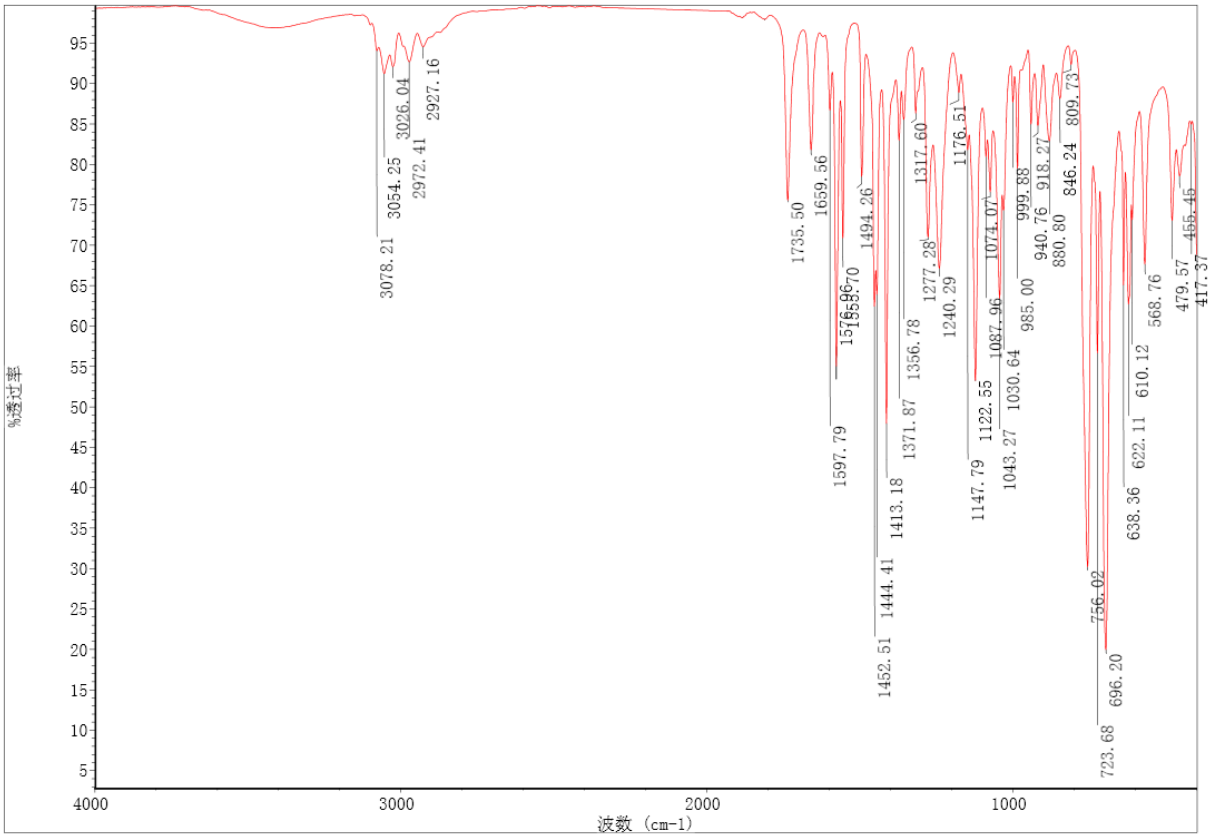
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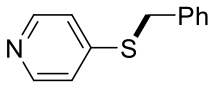
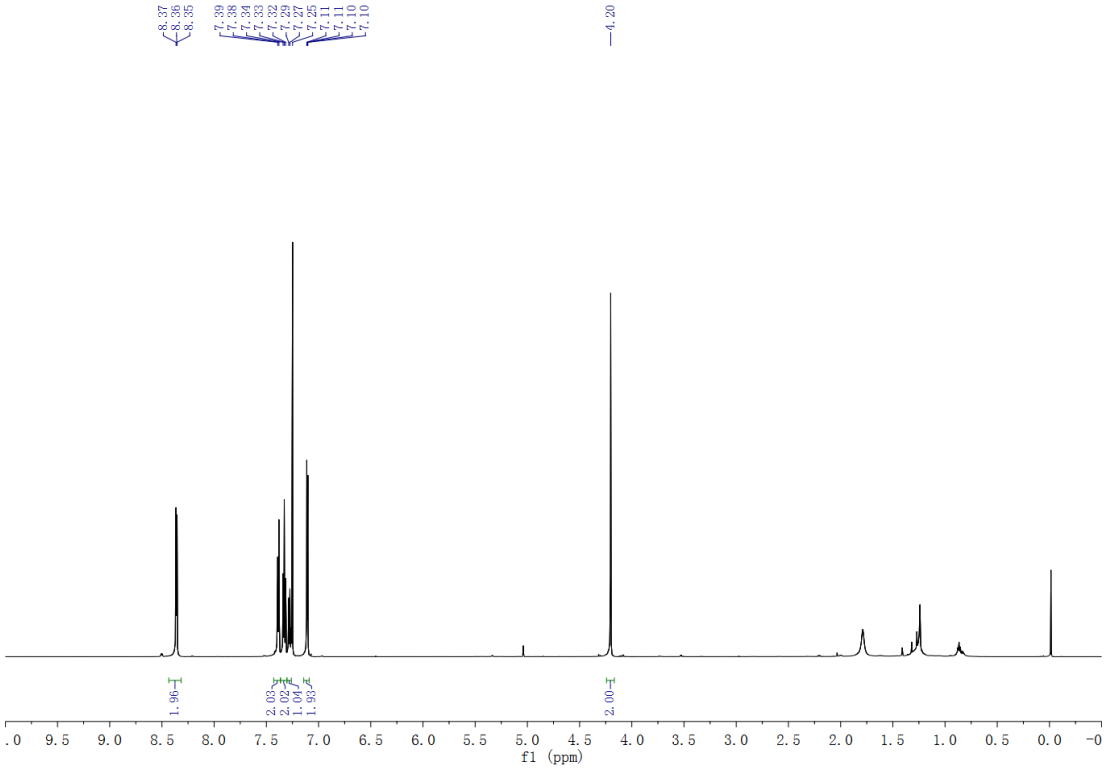
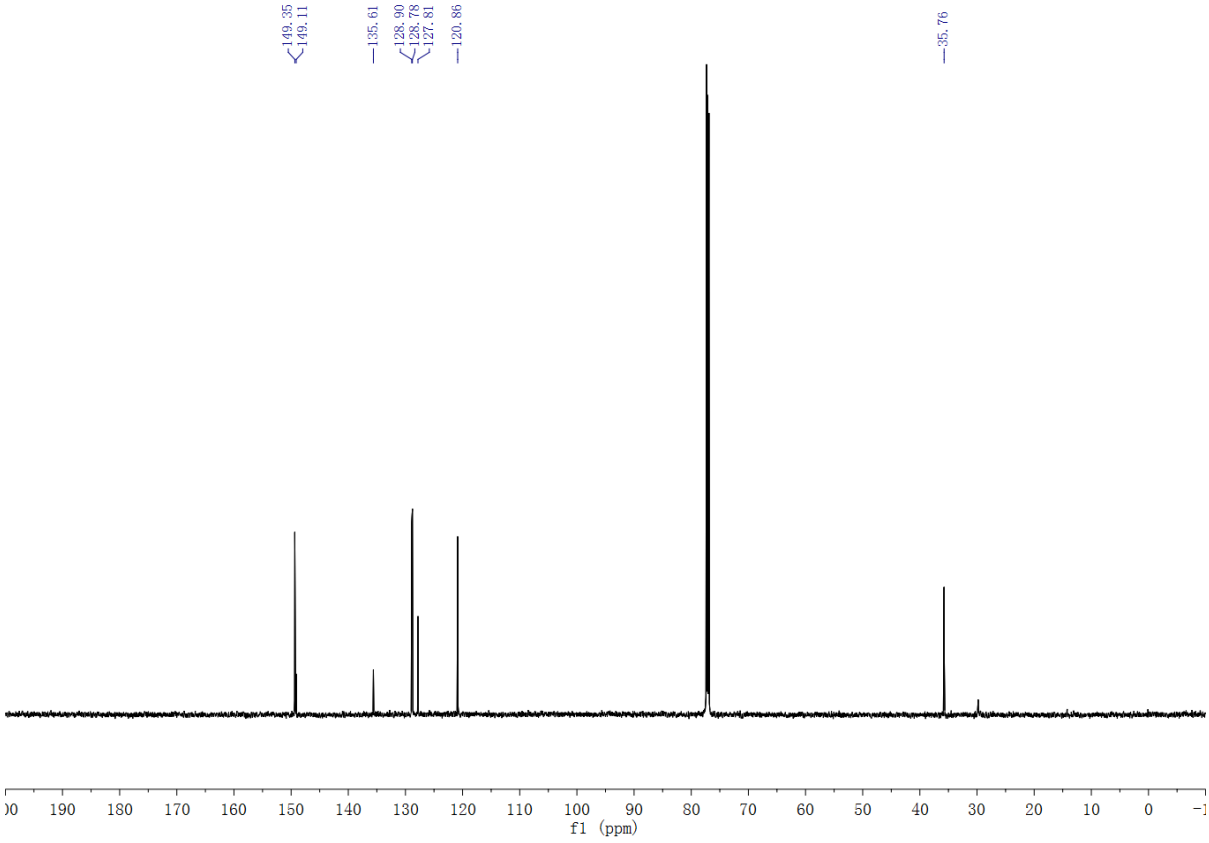


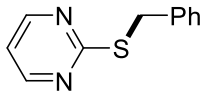
3ba

^{1}H NMR ($CDCl_3$, 600 M Hz)



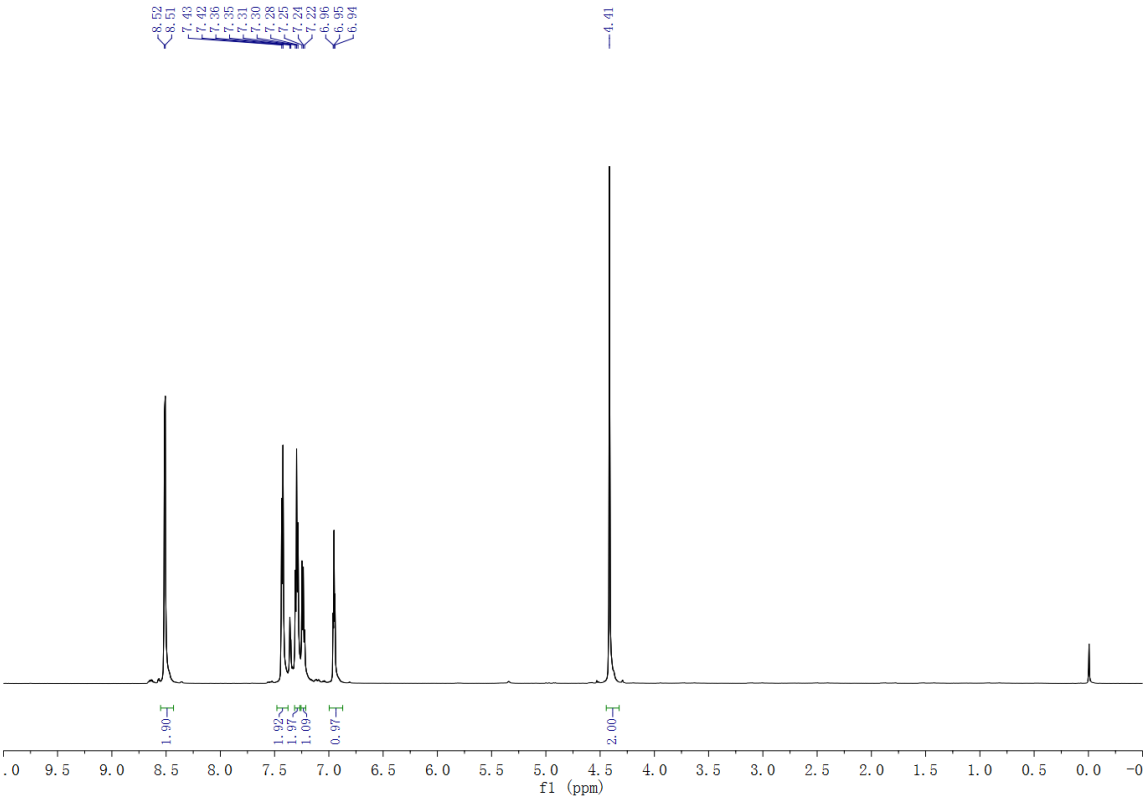
^{13}C NMR ($CDCl_3$, 150 M Hz)



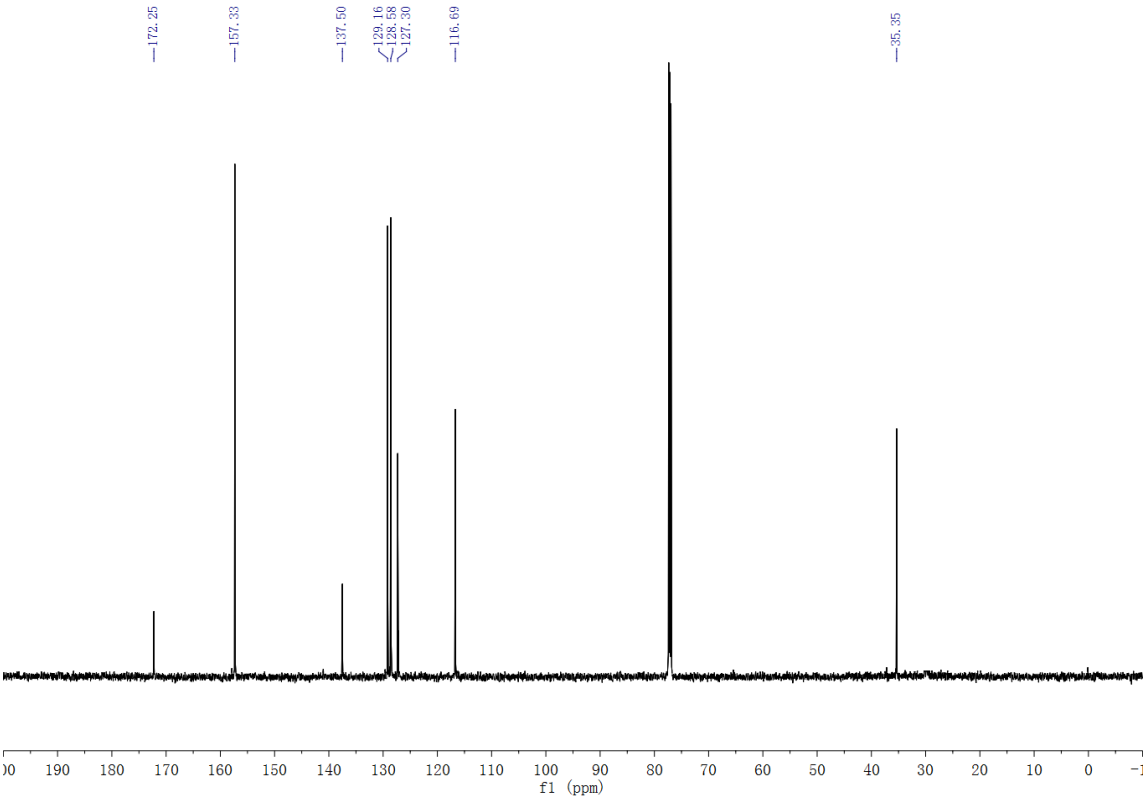


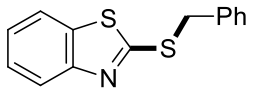
3ca

^{1}H NMR ($CDCl_3$, 600 M Hz)



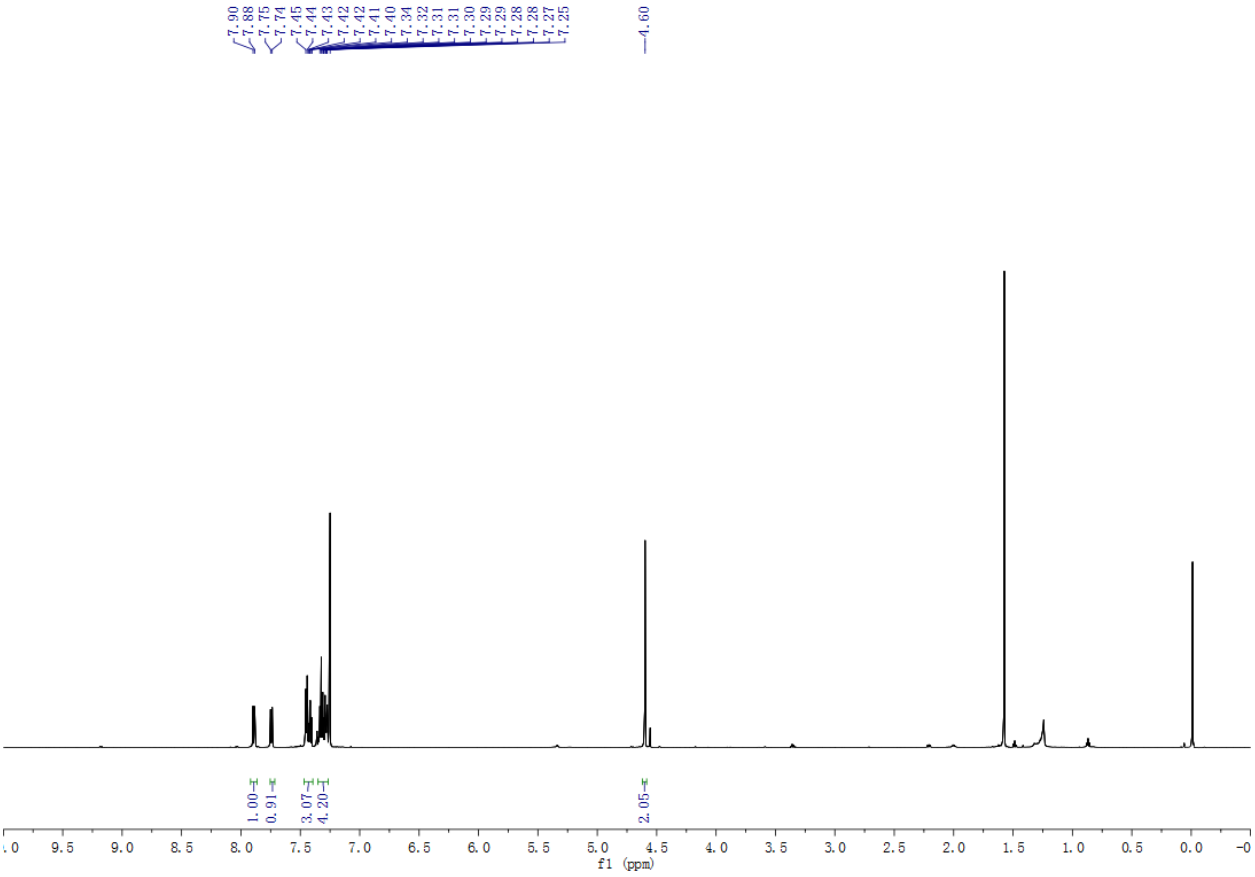
^{13}C NMR ($CDCl_3$, 150 M Hz)



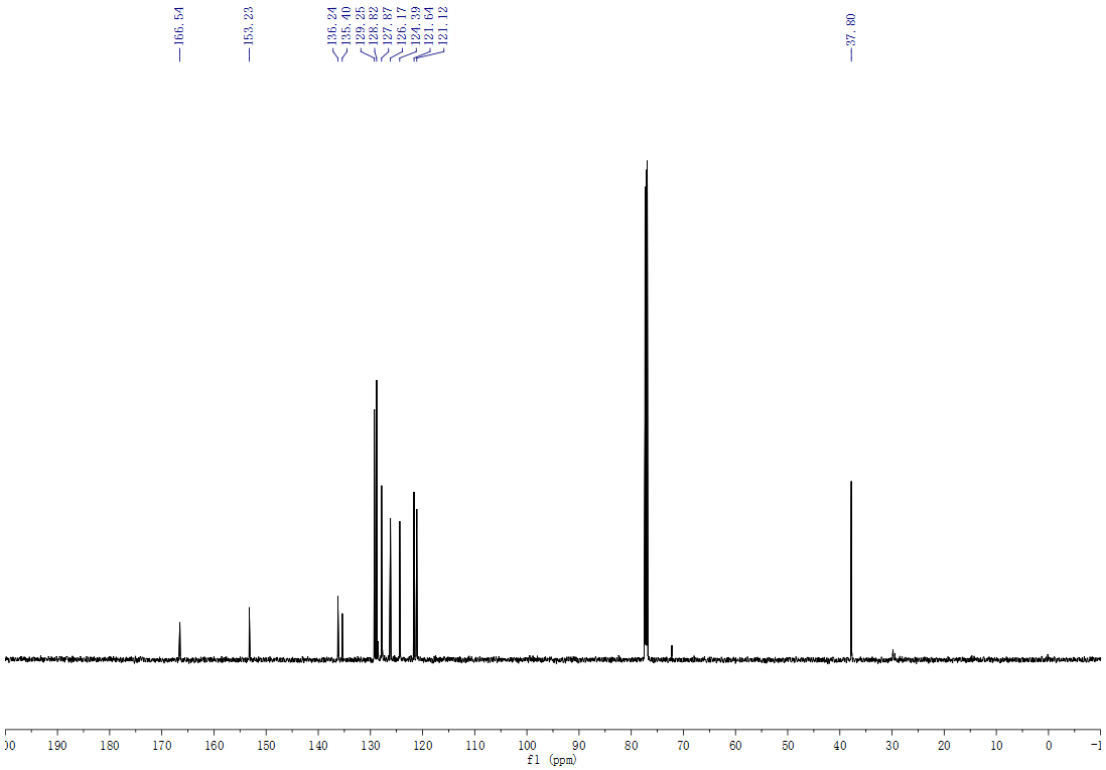


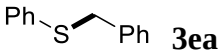
3da

^{1}H NMR ($CDCl_3$, 600 M Hz)



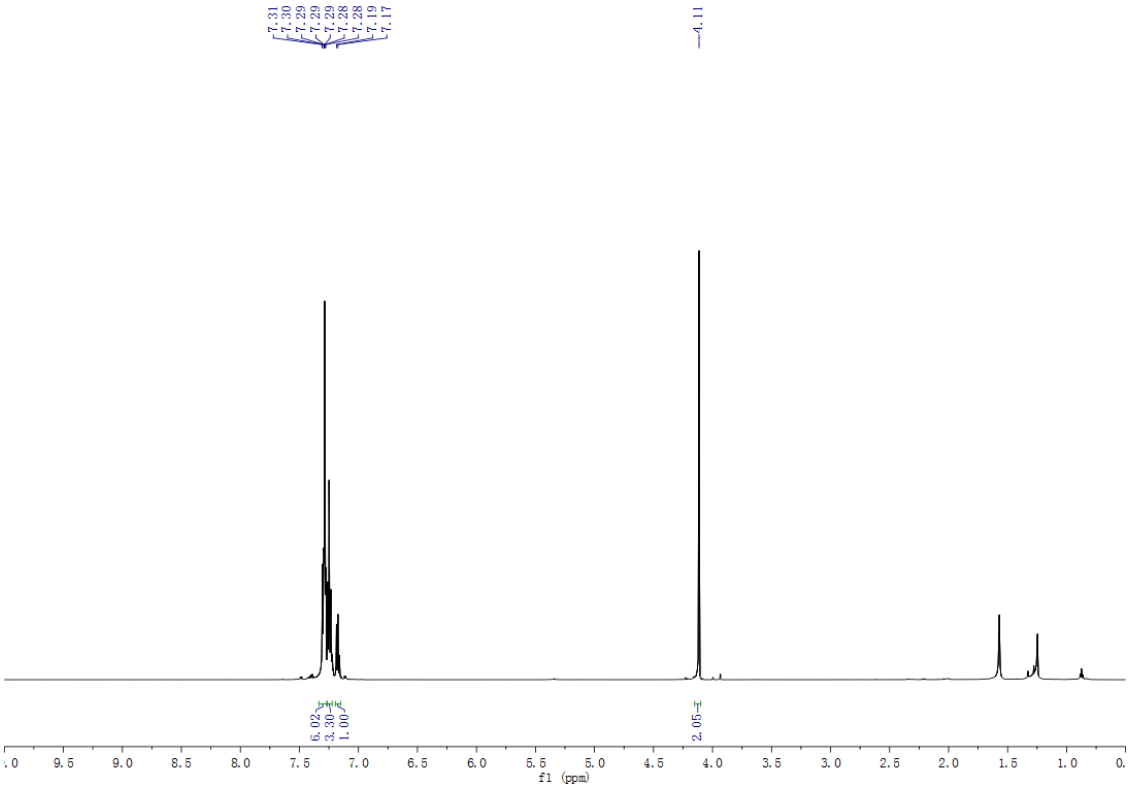
^{13}C NMR ($CDCl_3$, 150 M Hz)



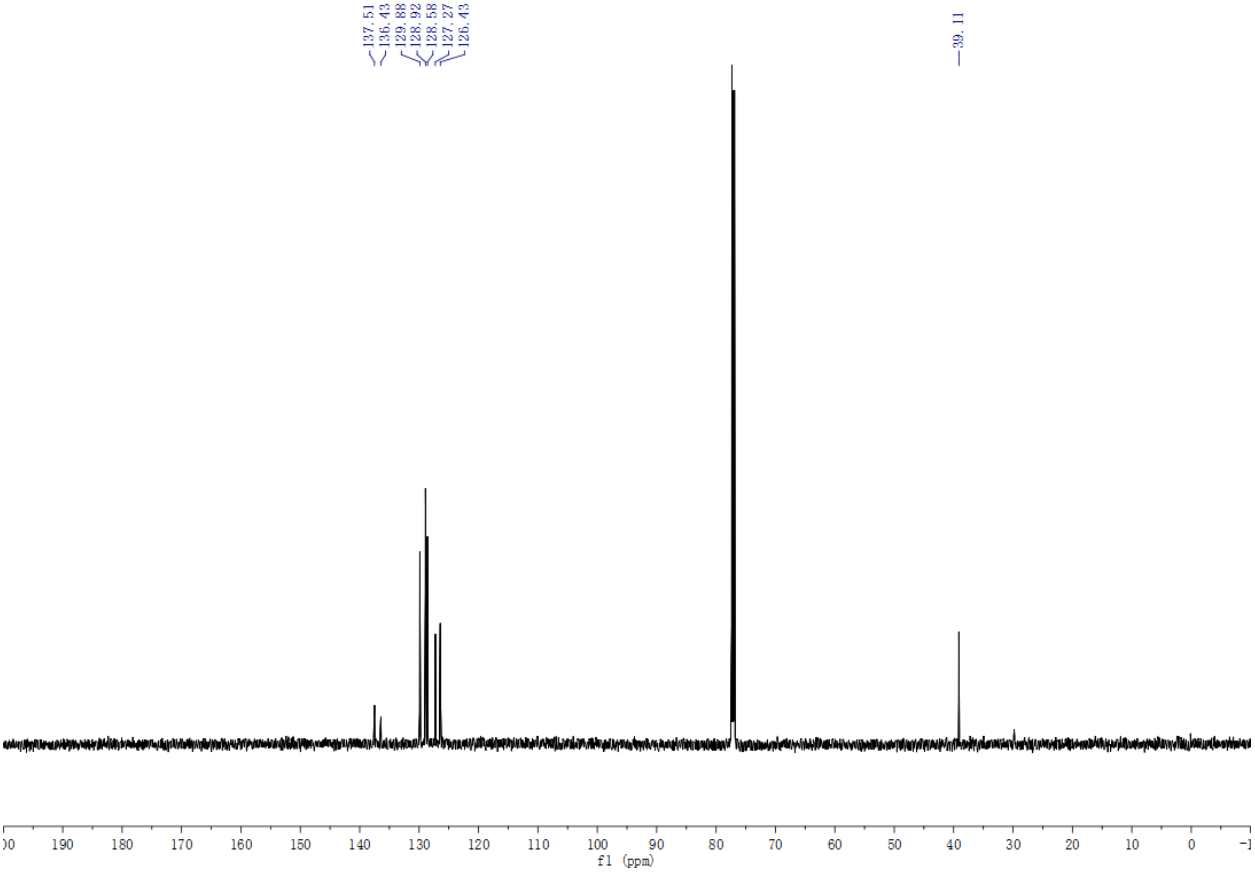


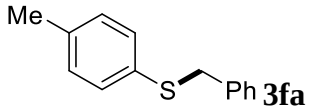
3ea

^{1}H NMR ($CDCl_3$, 600 M Hz)



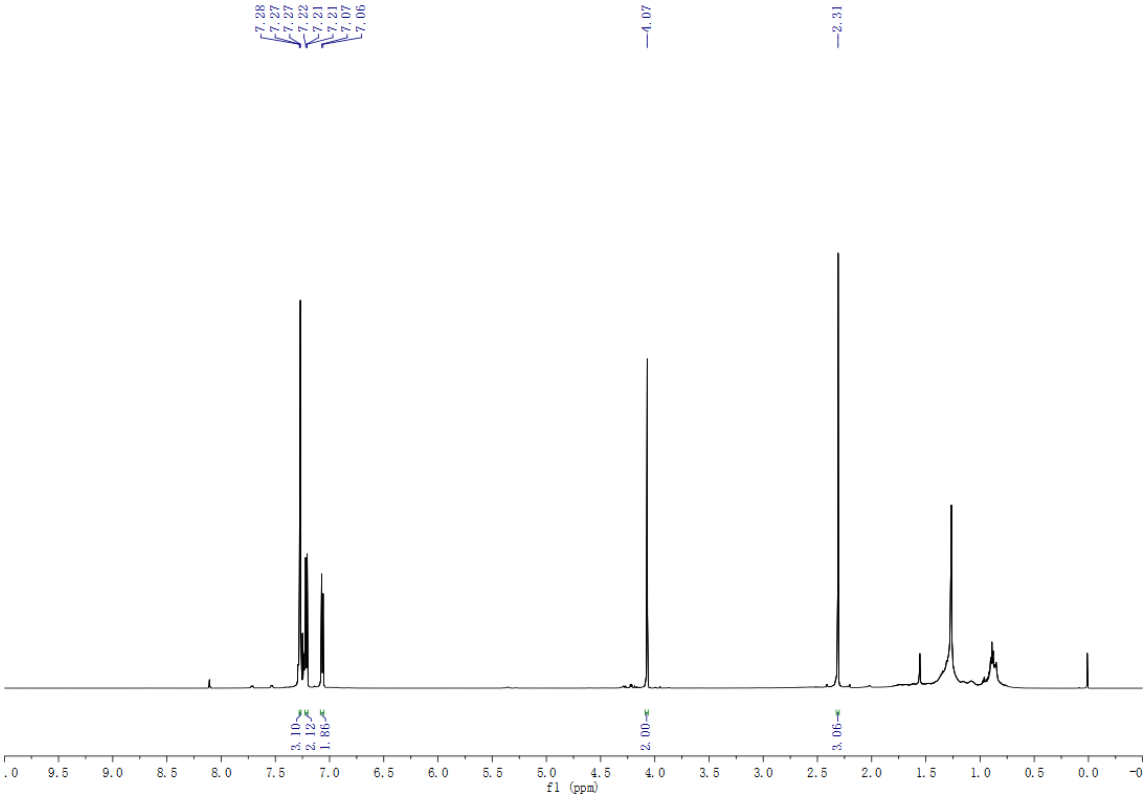
^{13}C NMR ($CDCl_3$, 150 M Hz)



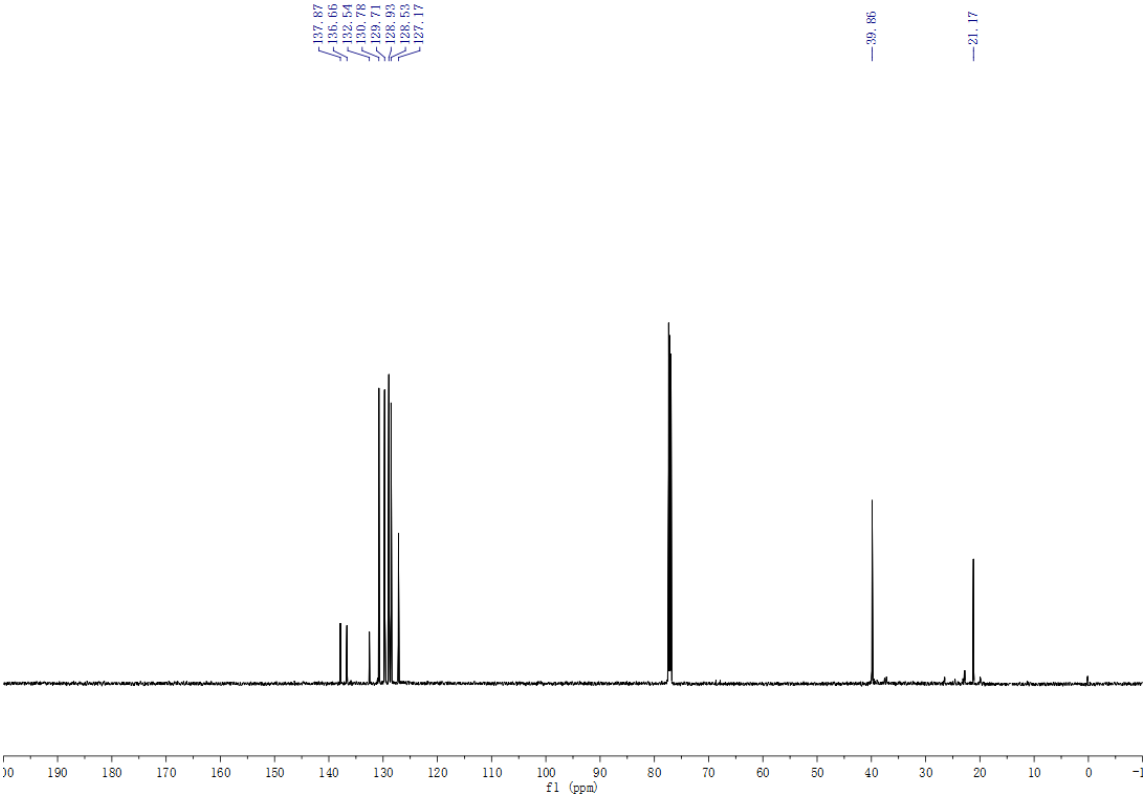


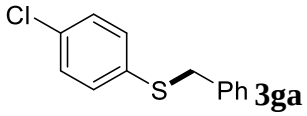
3fa

^{1}H NMR ($CDCl_3$, 600 M Hz)



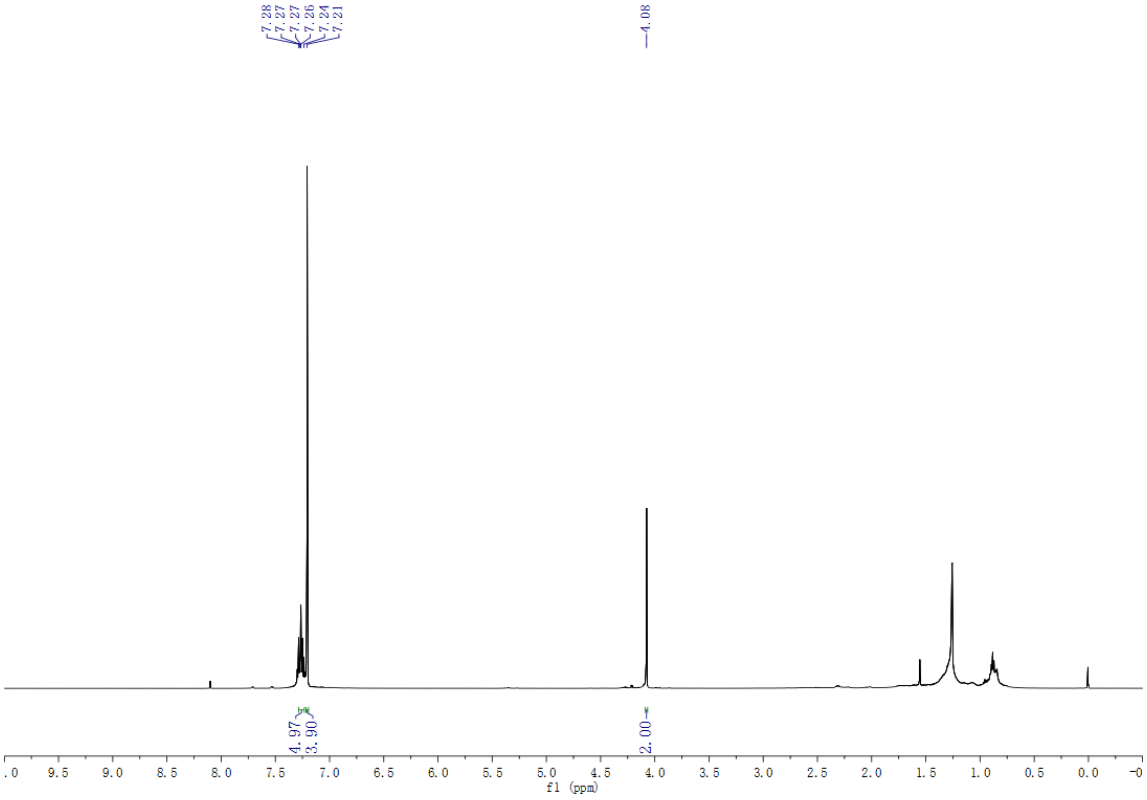
^{13}C NMR ($CDCl_3$, 150 M Hz)



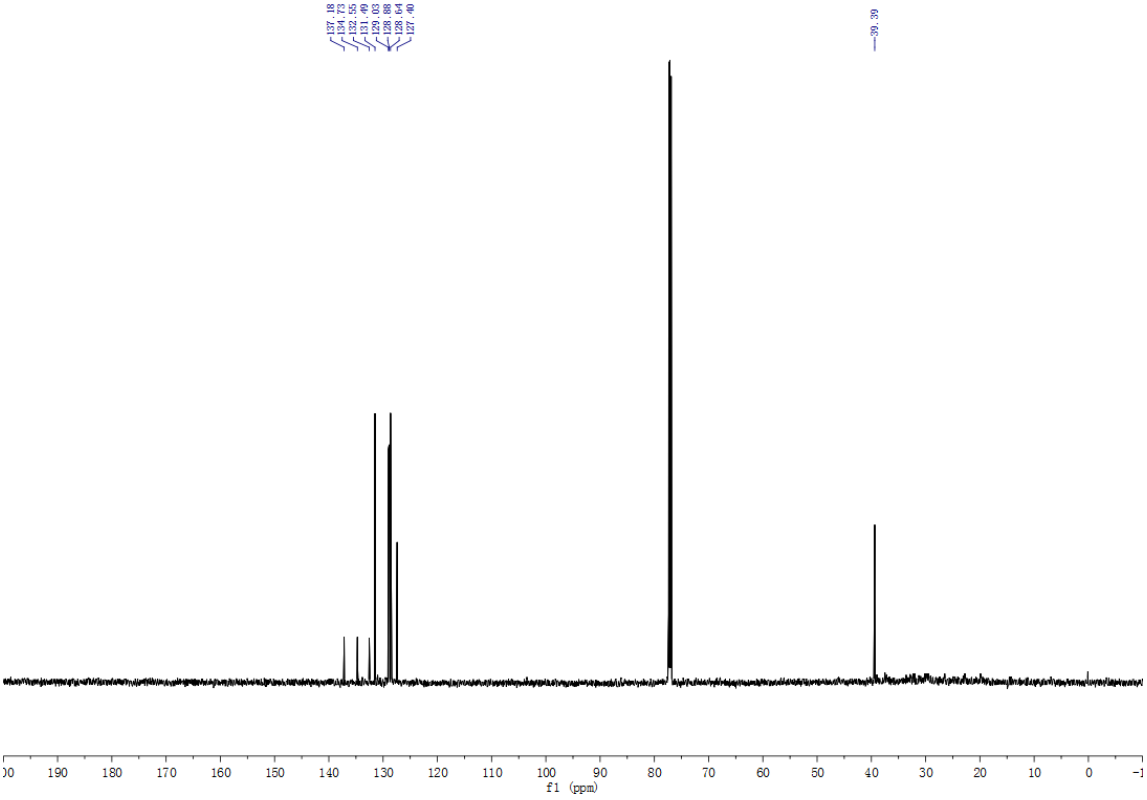


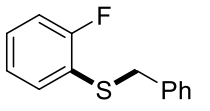
3ga

^{1}H NMR ($CDCl_3$, 600 M Hz)



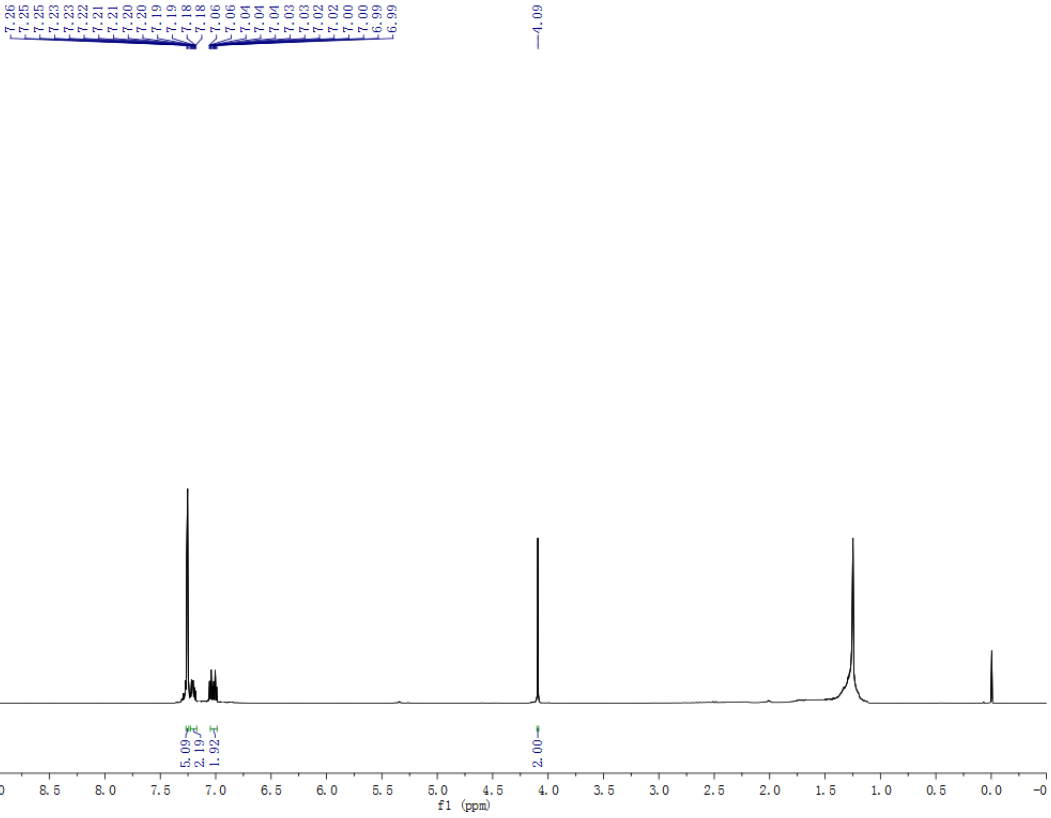
^{13}C NMR ($CDCl_3$, 150 M Hz)



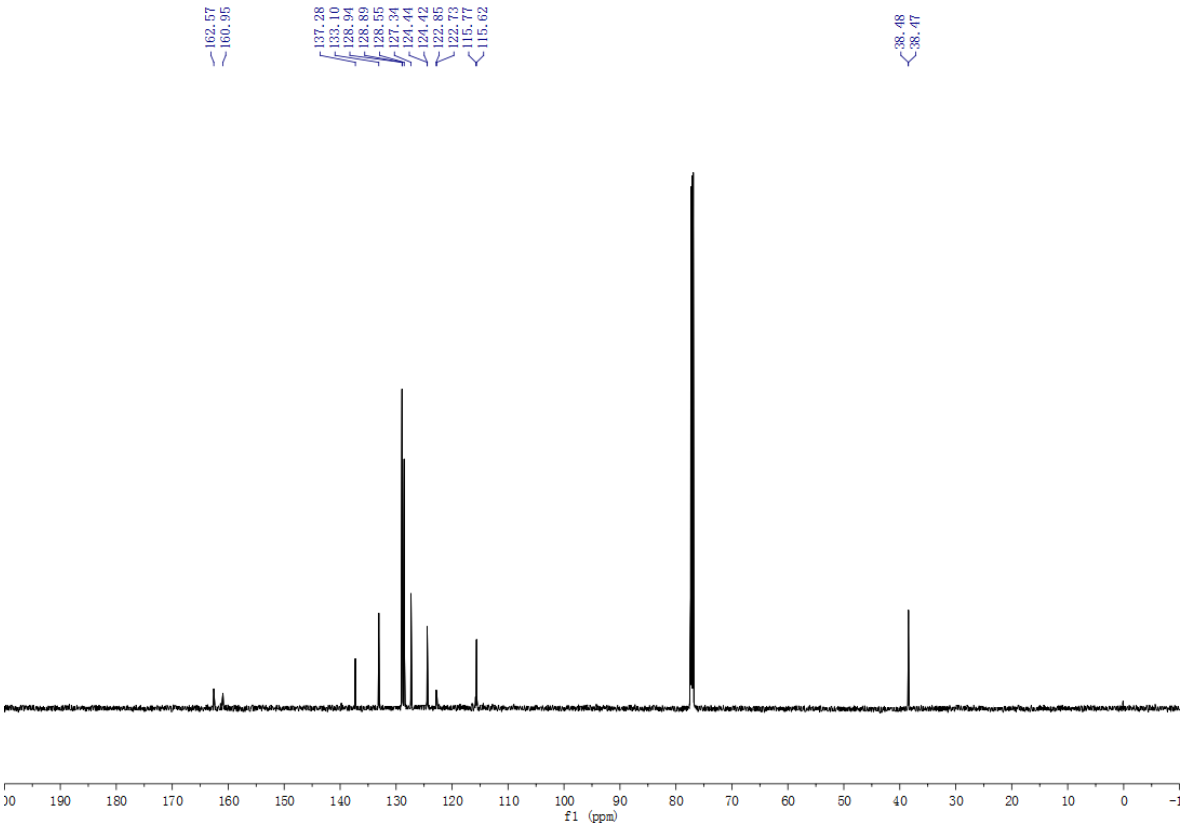


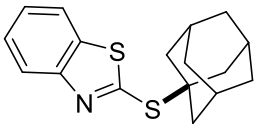
3ha

^{1}H NMR ($CDCl_3$, 600 M Hz)



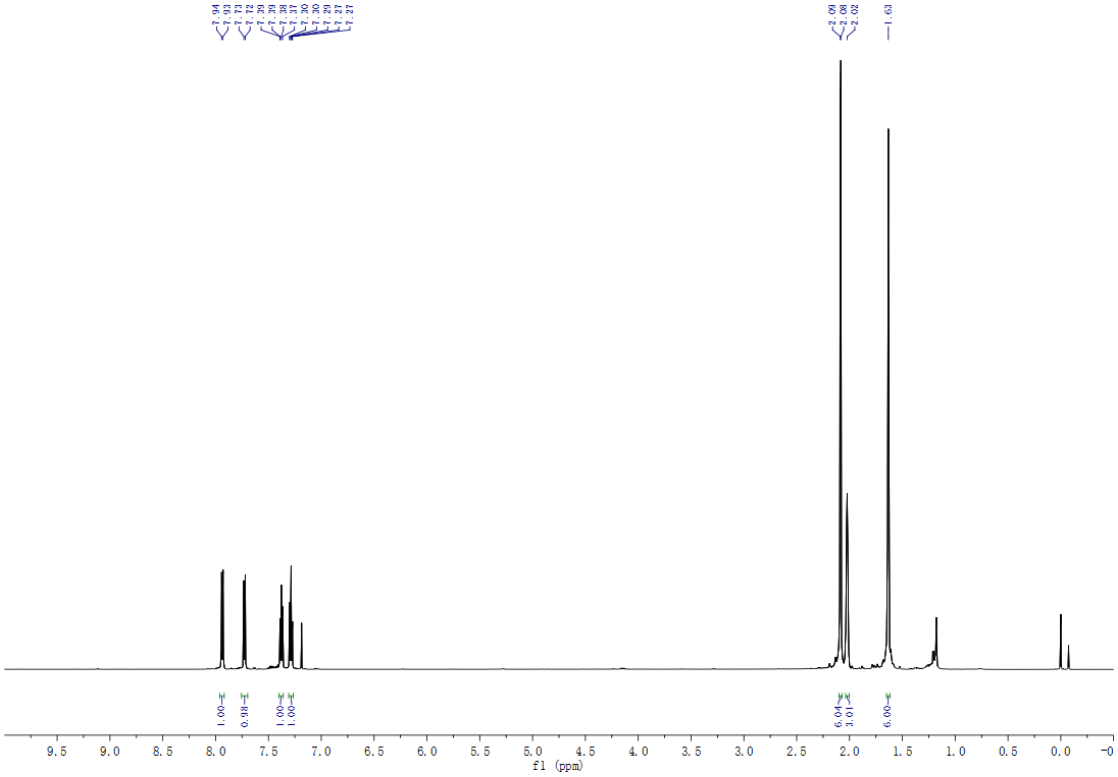
^{13}C NMR ($CDCl_3$, 150 M Hz)



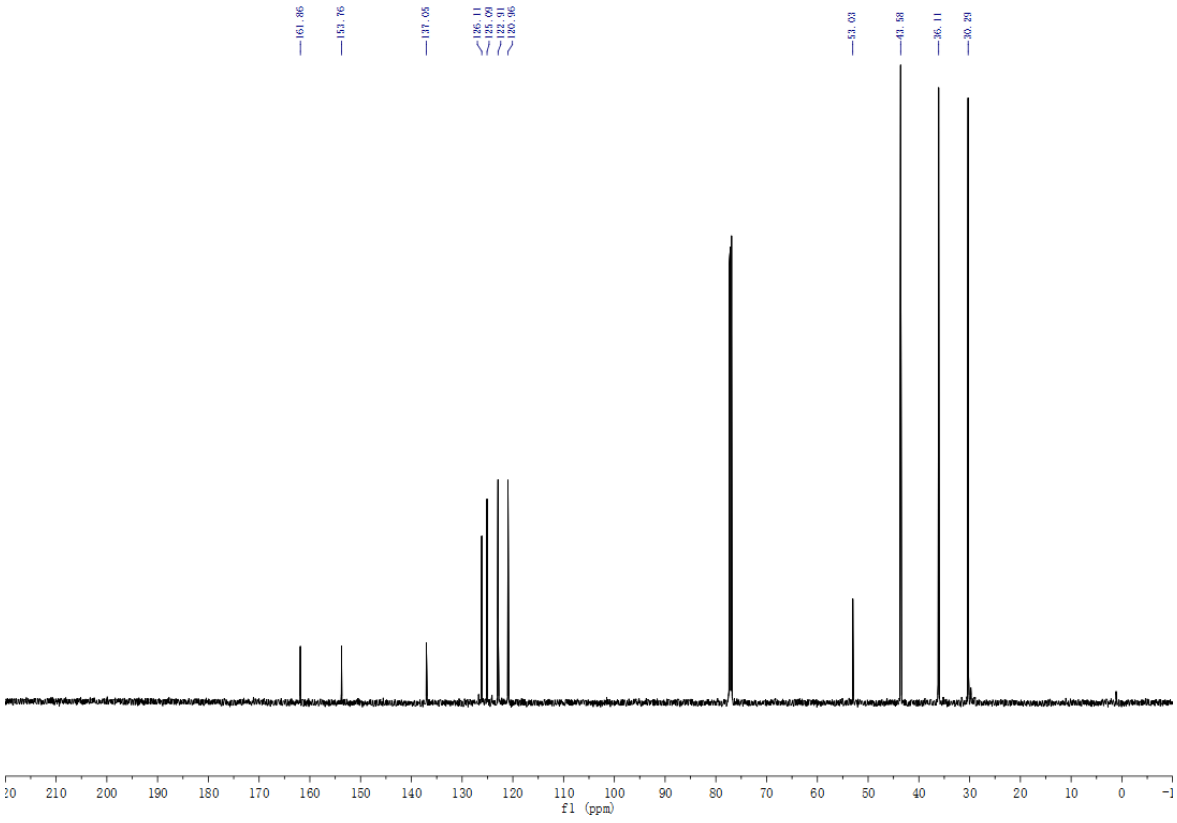


3dK

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)



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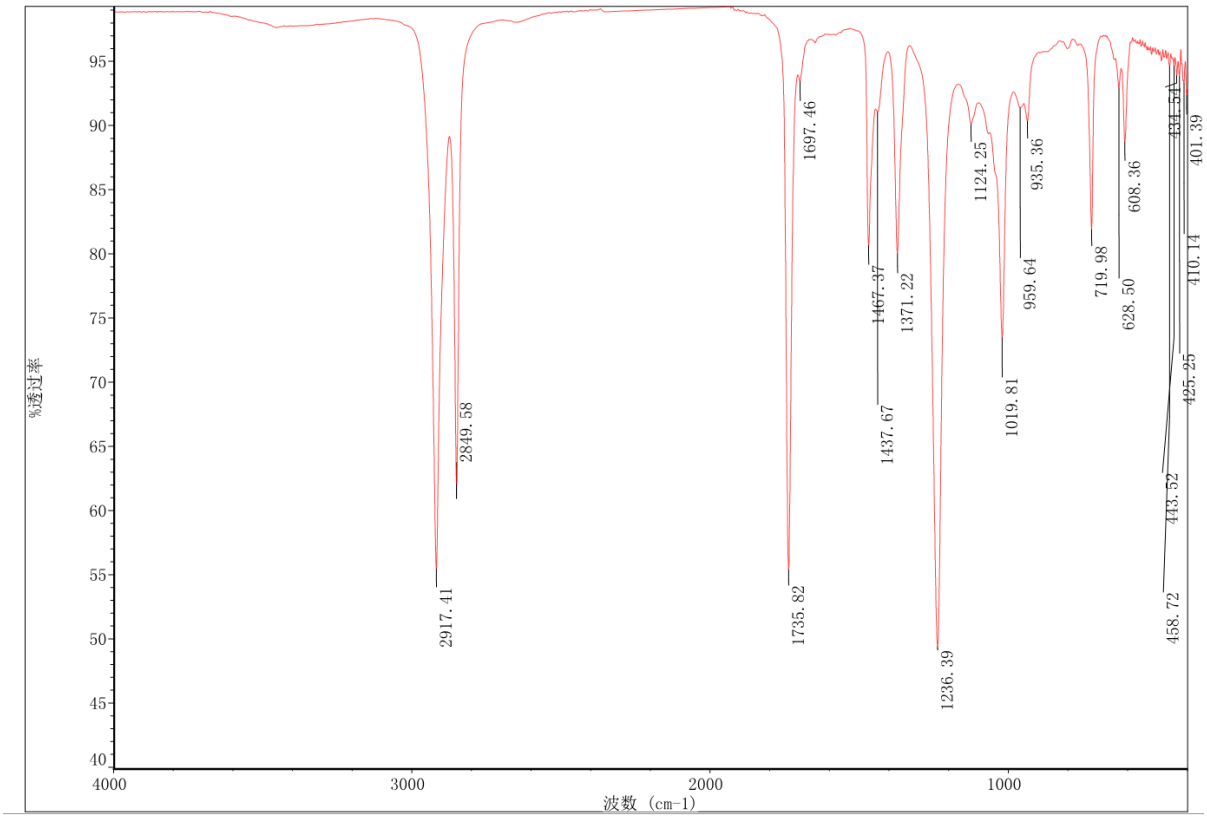
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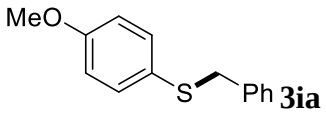
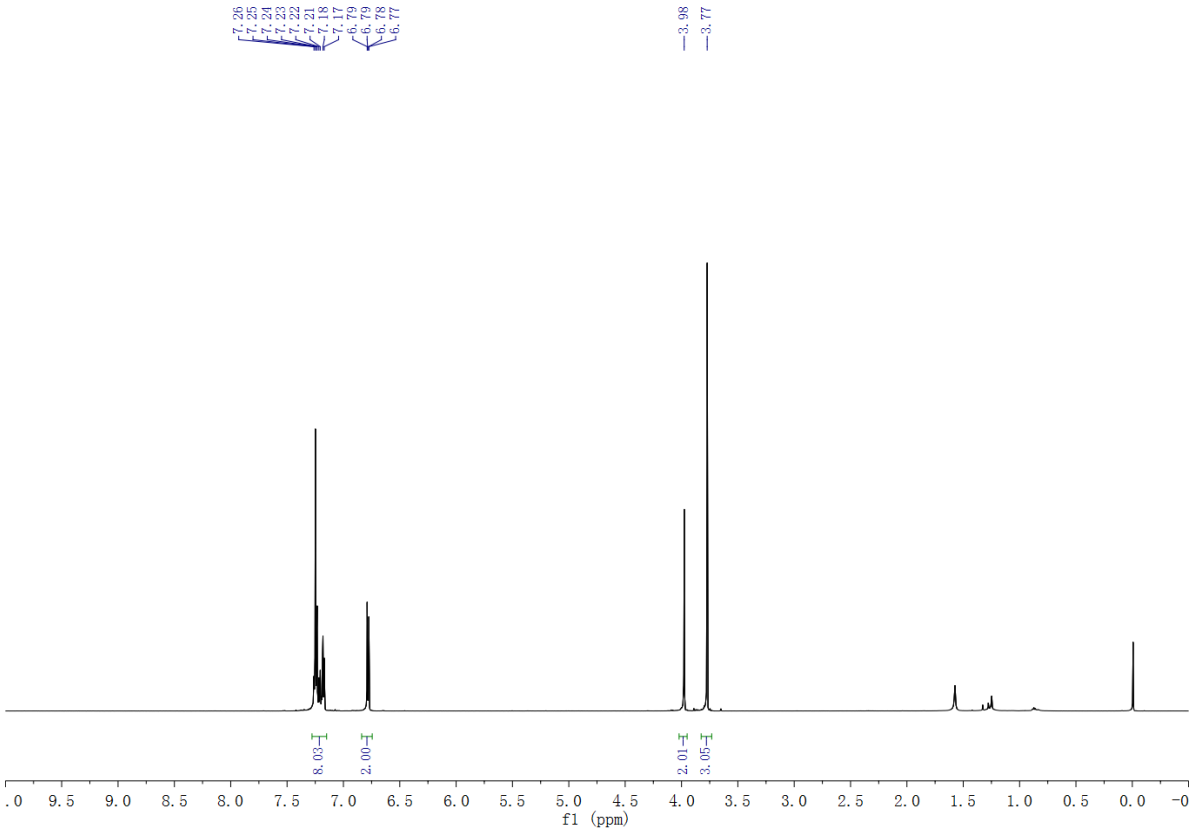
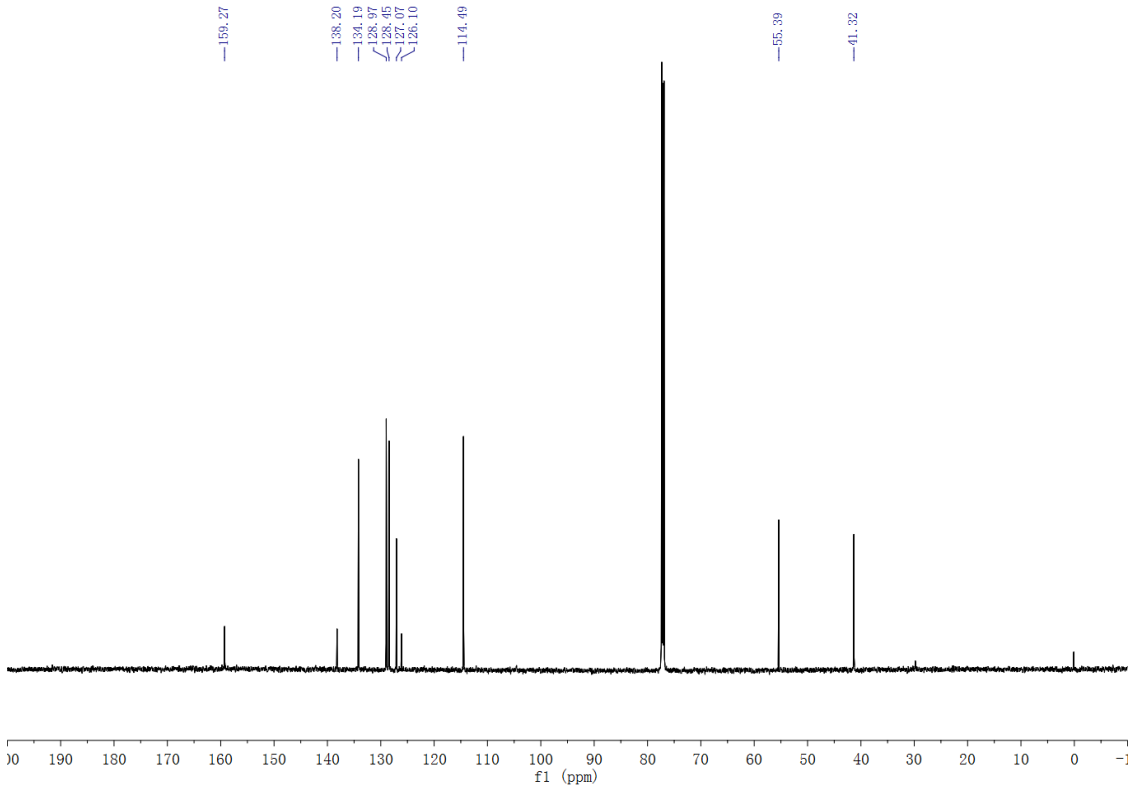


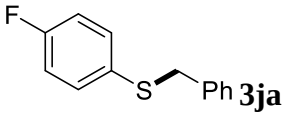
3ia

^{1}H NMR ($CDCl_3$, 600 M Hz)



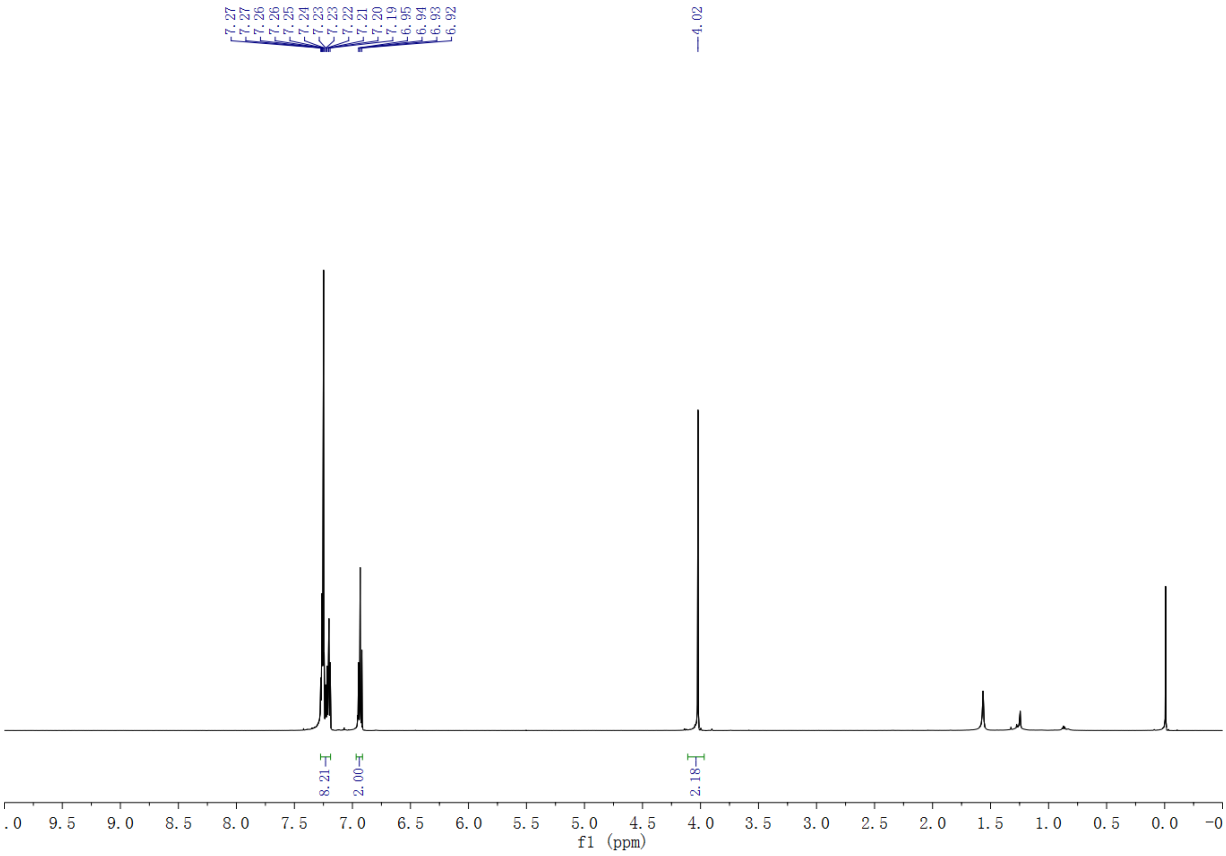
^{13}C NMR ($CDCl_3$, 150 M Hz)



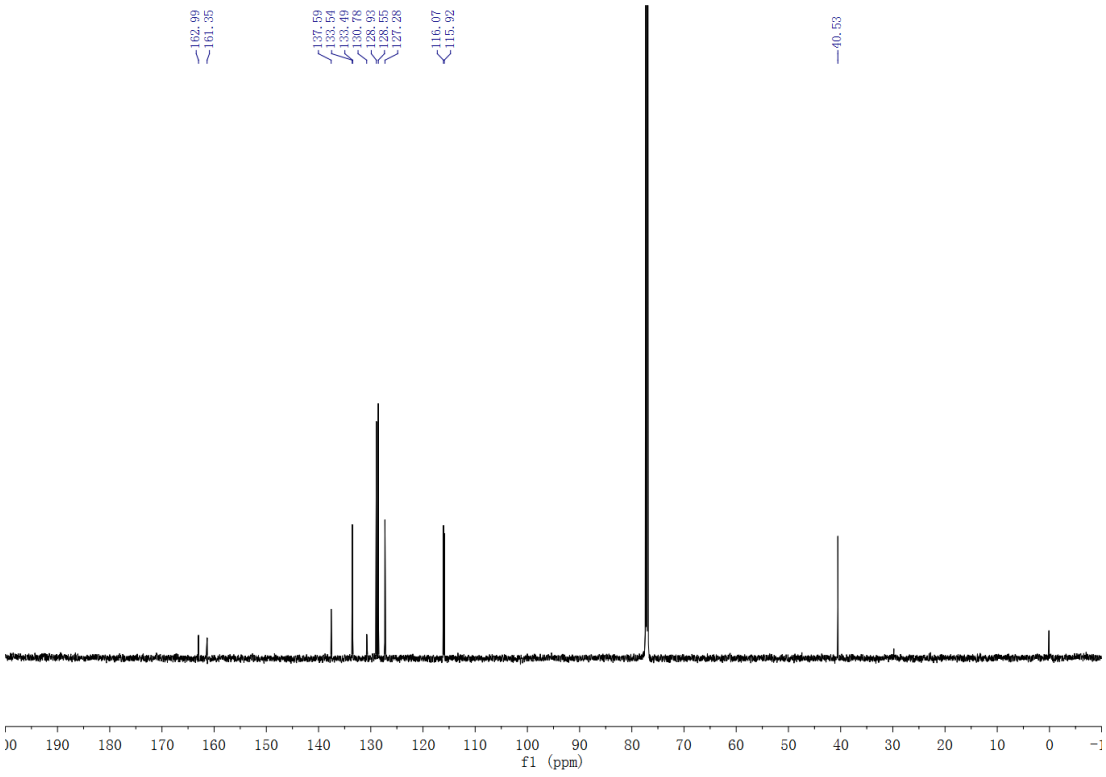


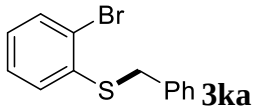
3ja

^{1}H NMR ($CDCl_3$, 600 M Hz)



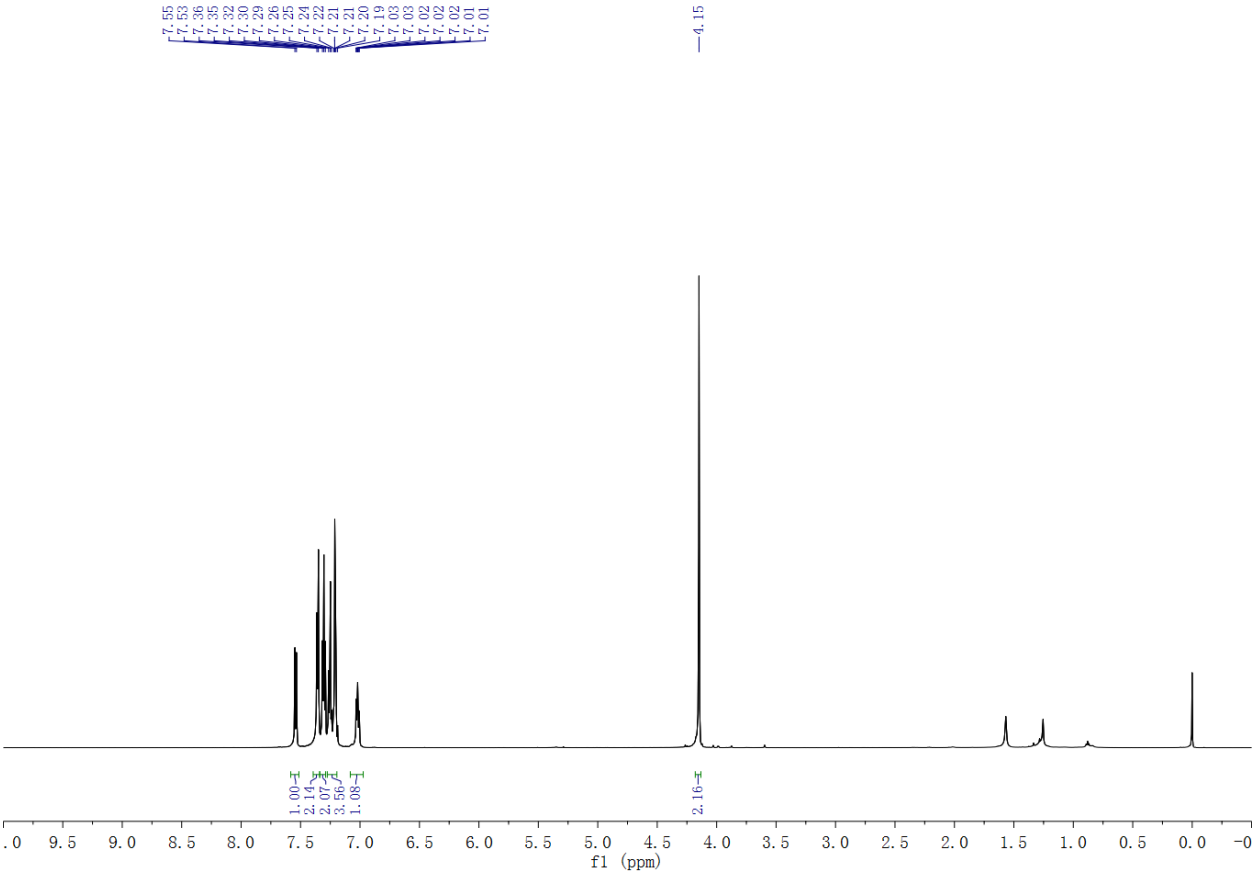
^{13}C NMR ($CDCl_3$, 150 M Hz)



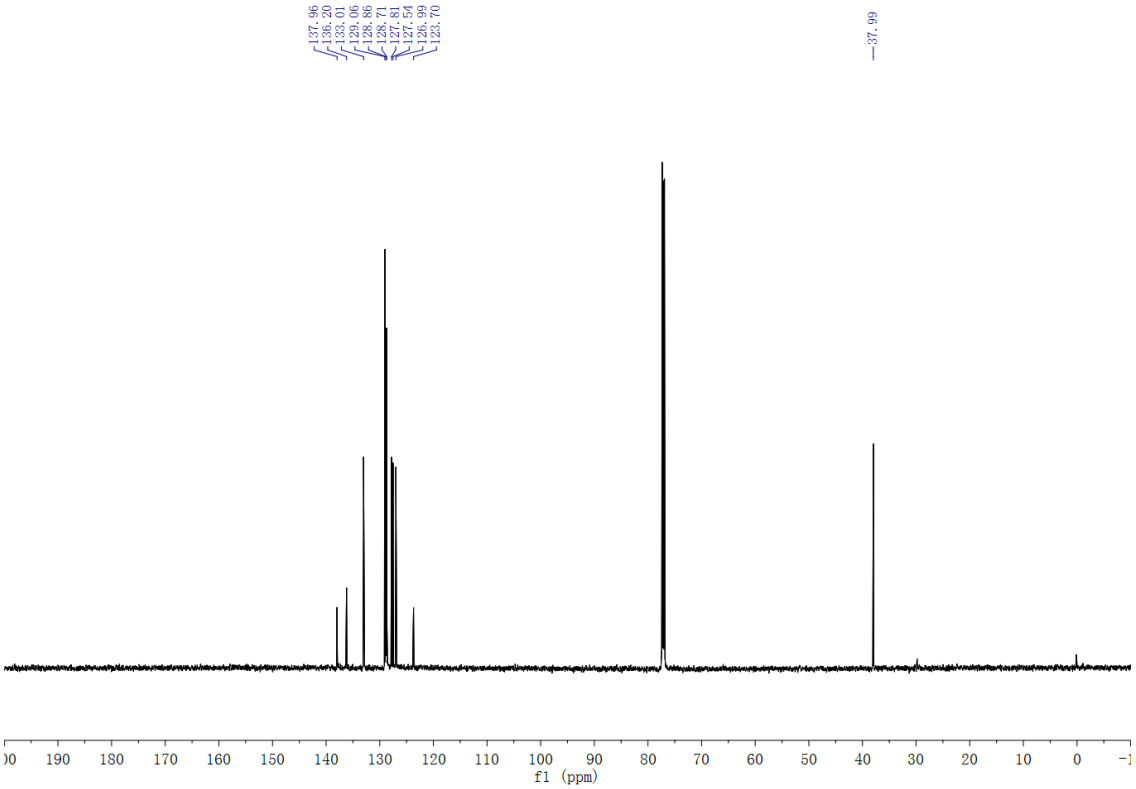


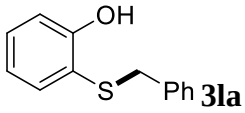
3ka

^{1}H NMR ($CDCl_3$, 600 M Hz)



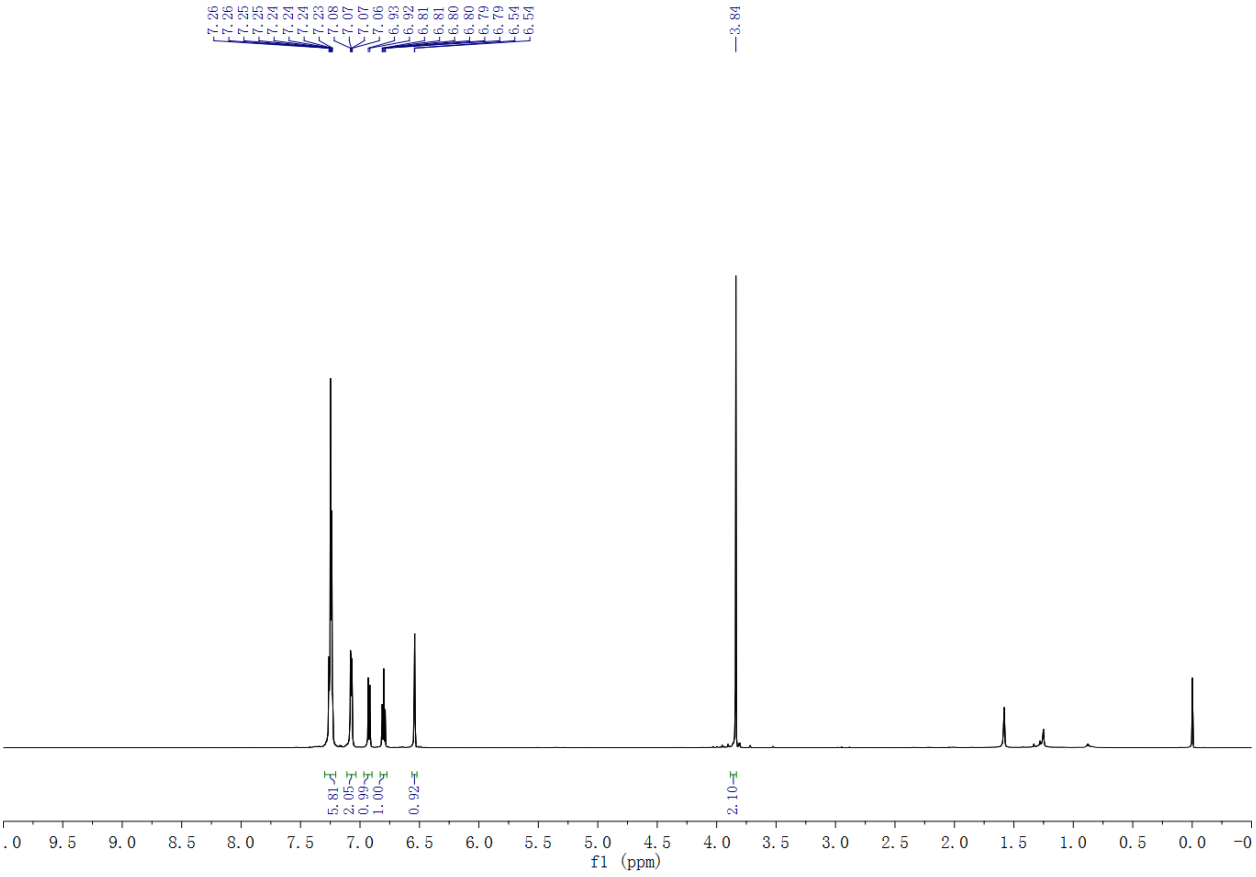
^{13}C NMR ($CDCl_3$, 150 M Hz)



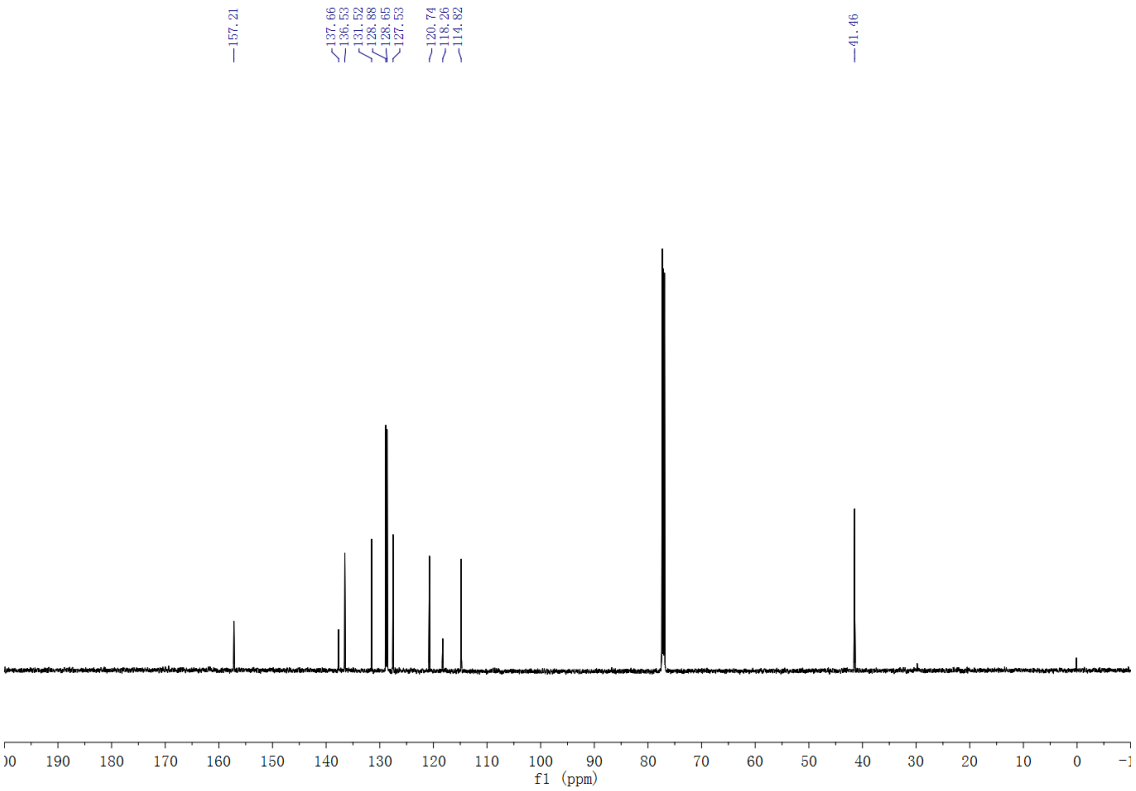


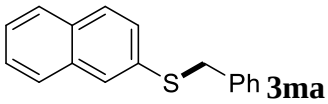
3la

^{1}H NMR ($CDCl_3$, 600 M Hz)



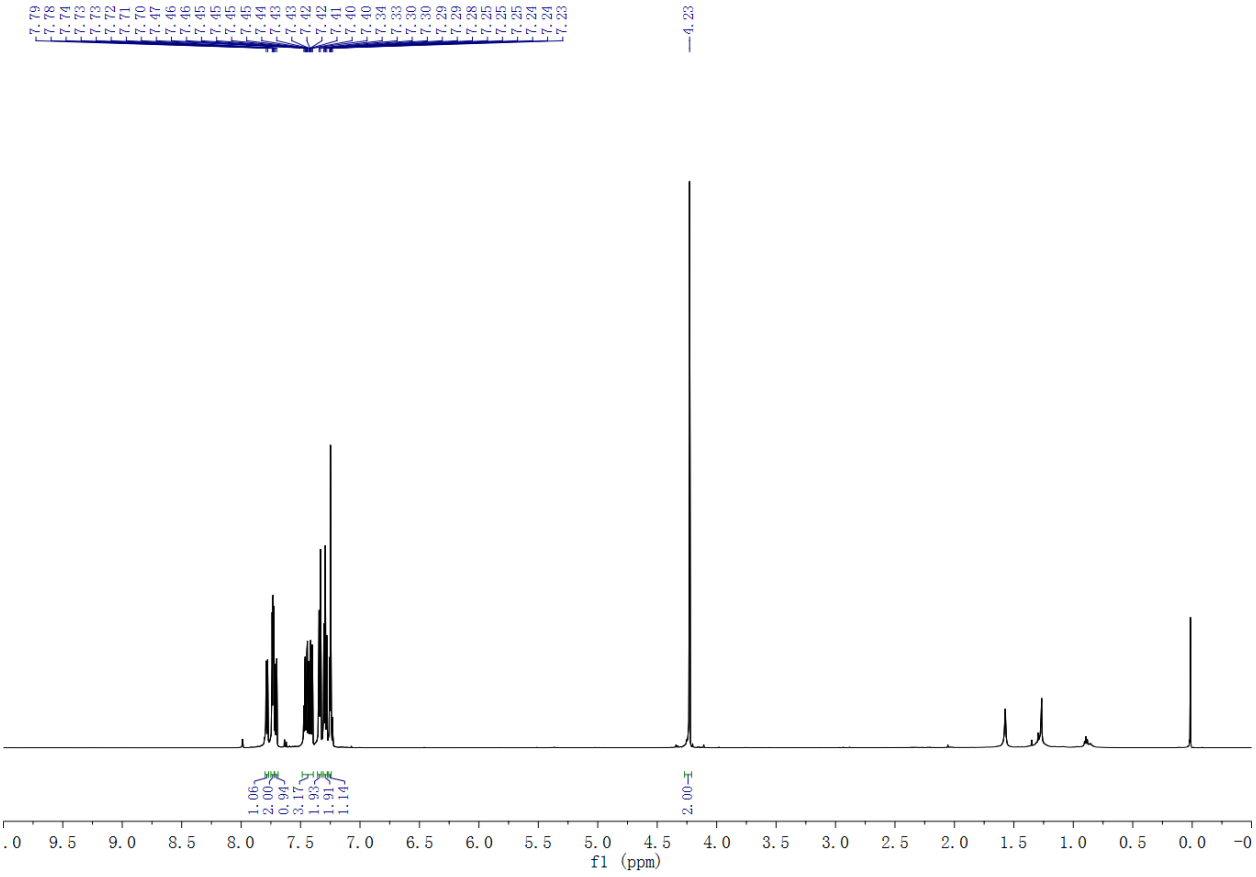
^{13}C NMR ($CDCl_3$, 150 M Hz)



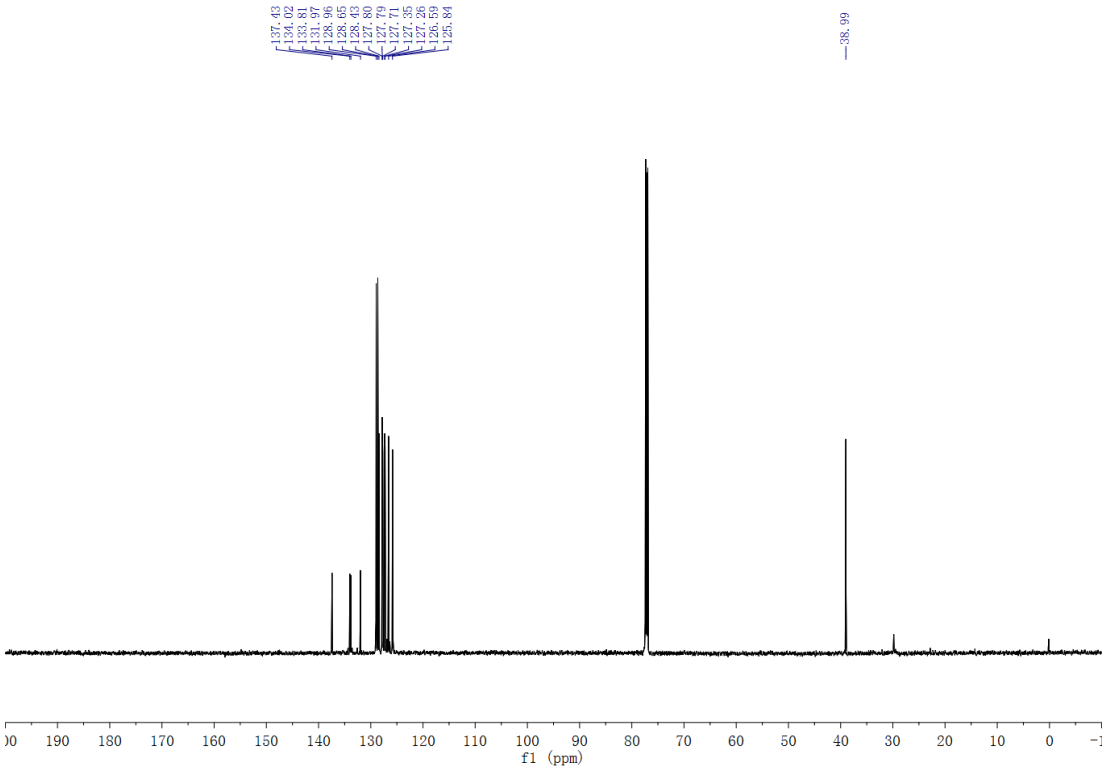


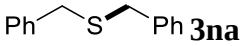
3ma

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)





3na

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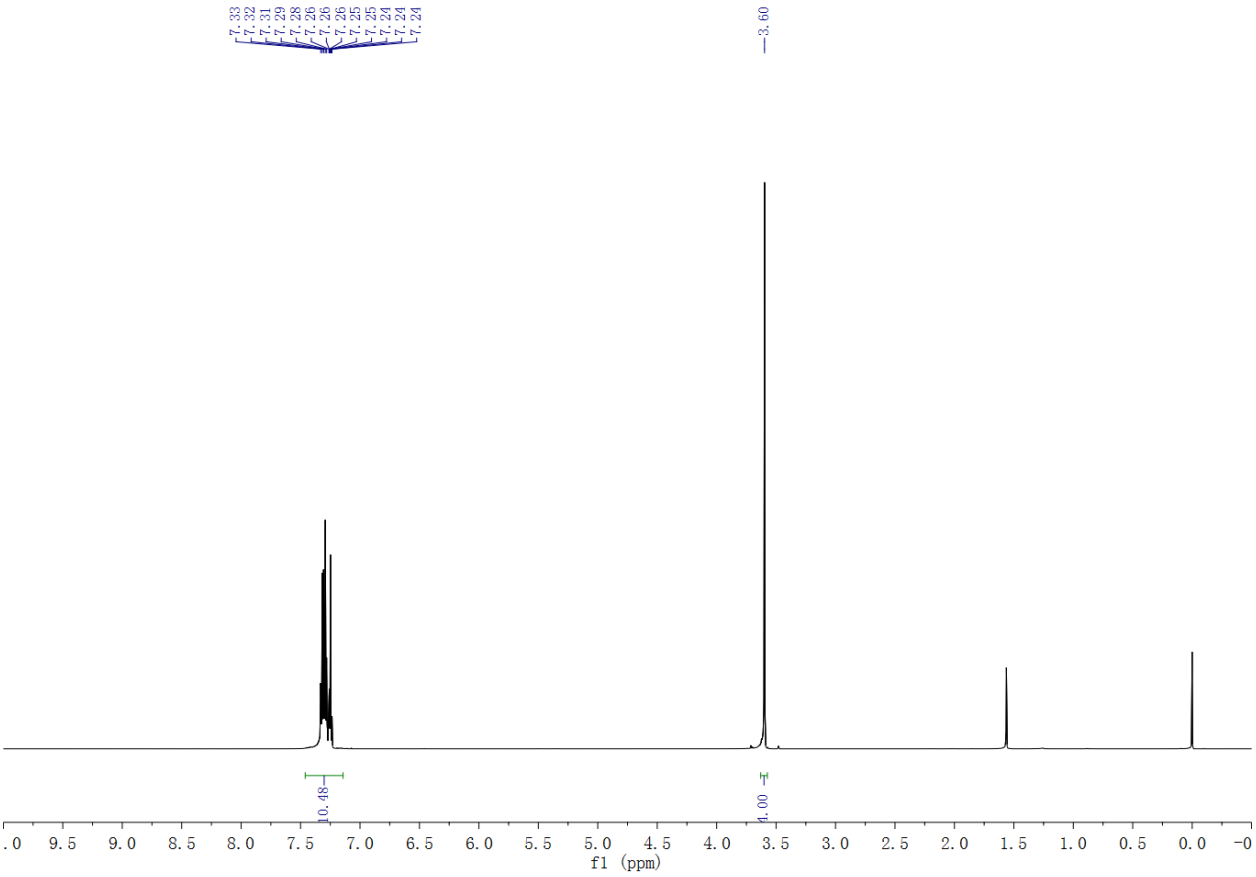
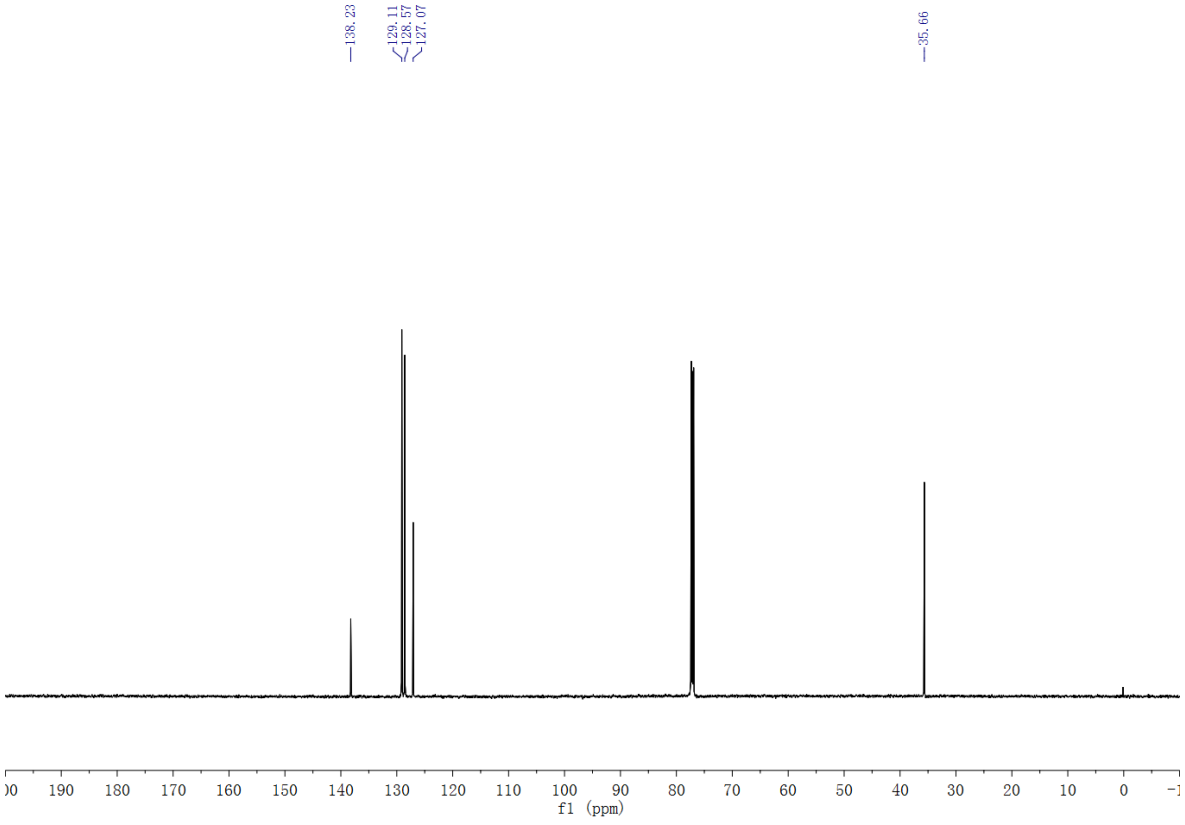
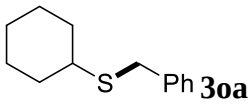


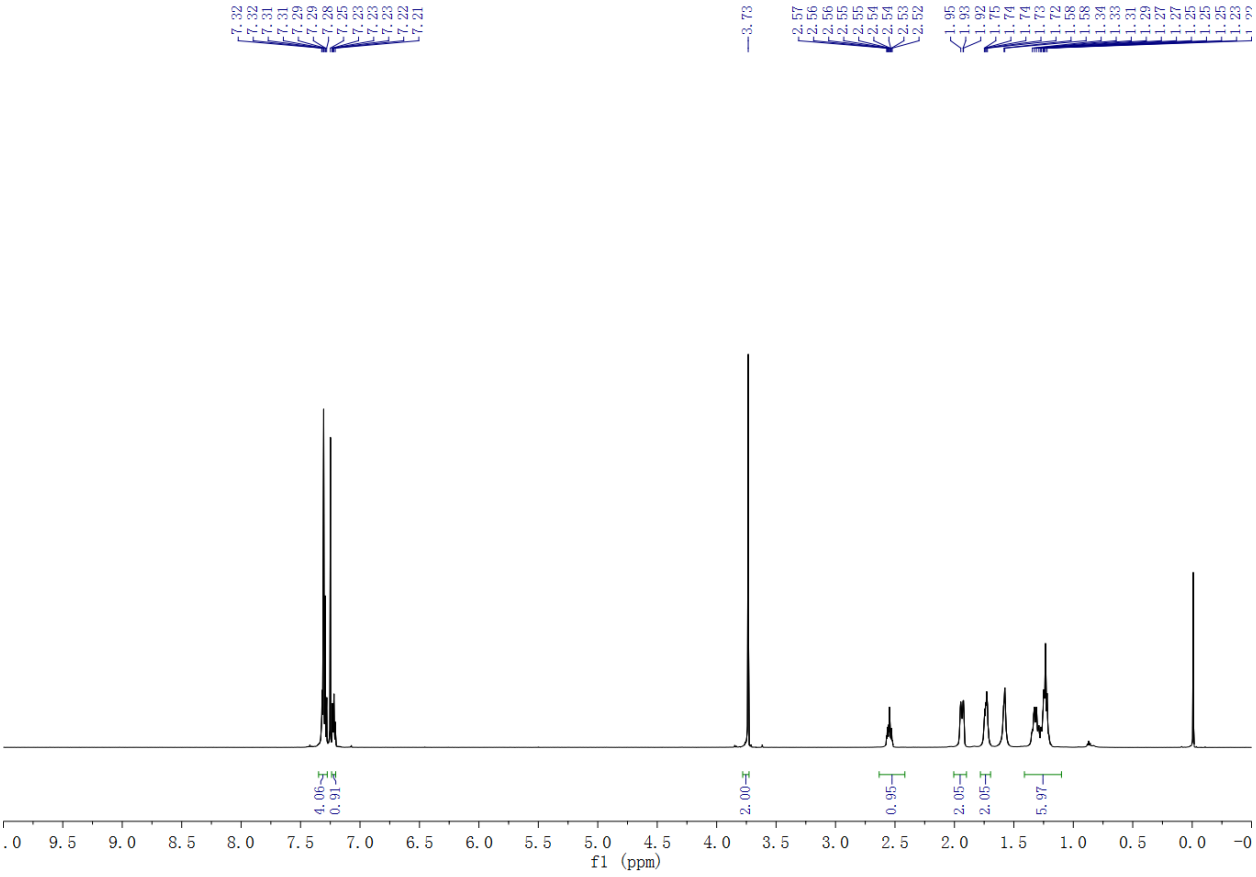
^{13}C NMR ($CDCl_3$, 150 M Hz)



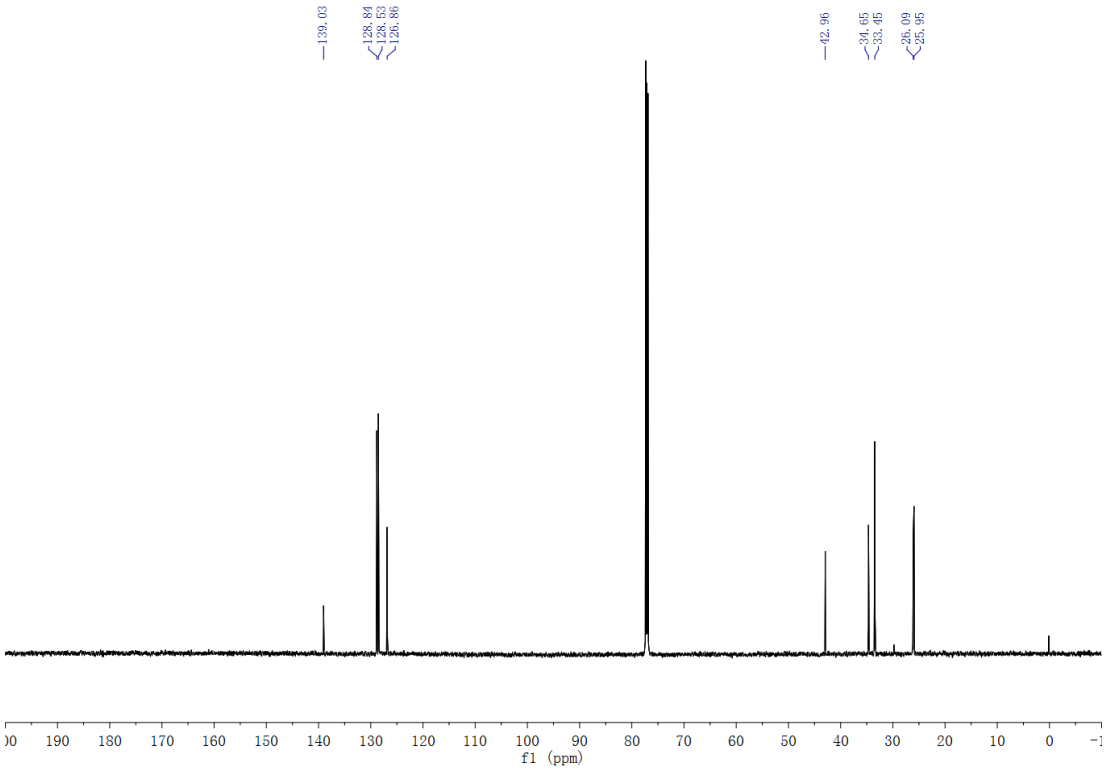


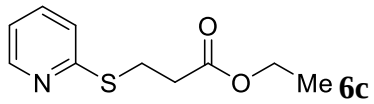
3oa

^{1}H NMR ($CDCl_3$, 600 M Hz)



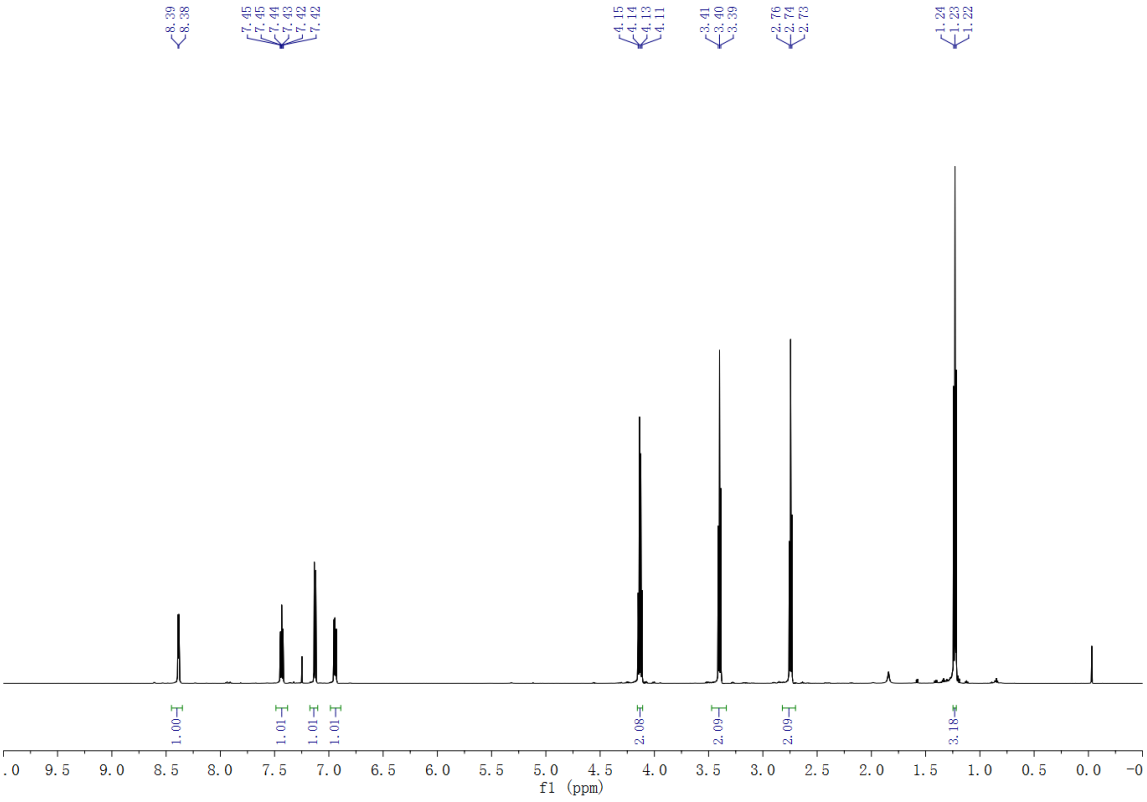
^{13}C NMR ($CDCl_3$, 150 M Hz)



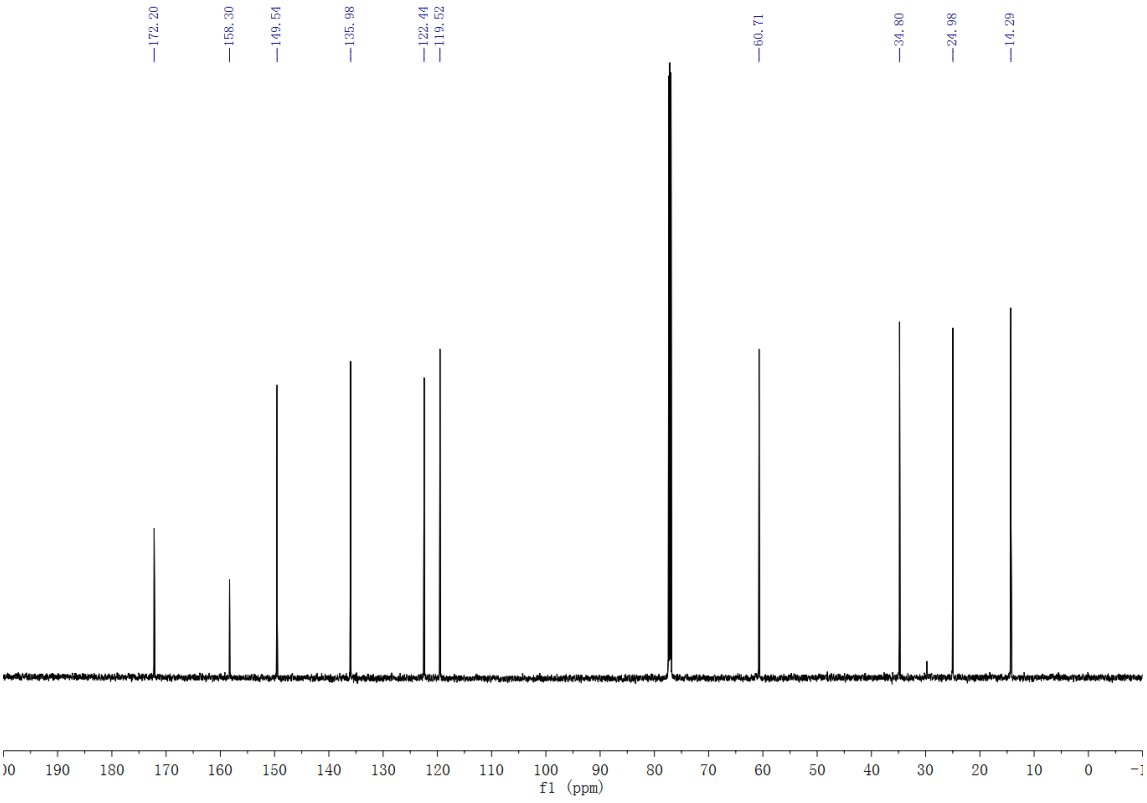


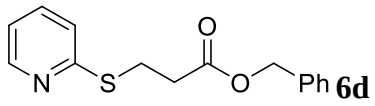
6c

^{1}H NMR ($CDCl_3$, 600 M Hz)



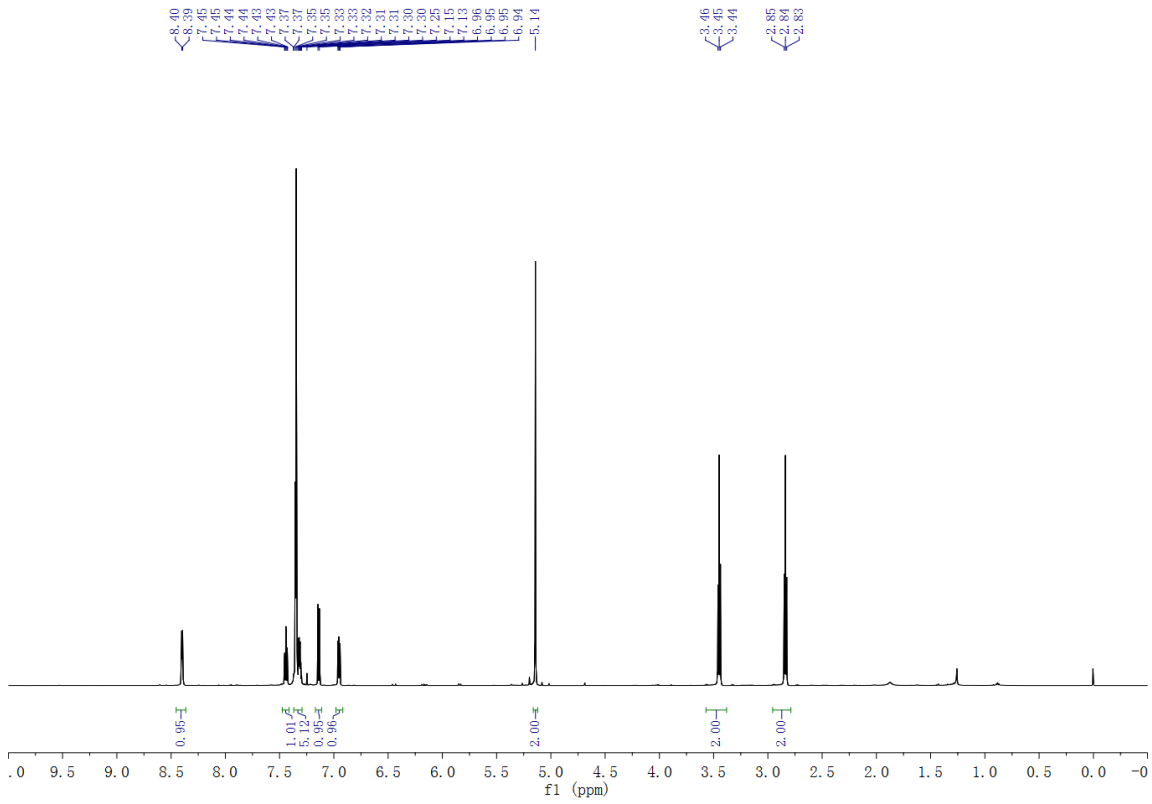
^{13}C NMR ($CDCl_3$, 150 M Hz)



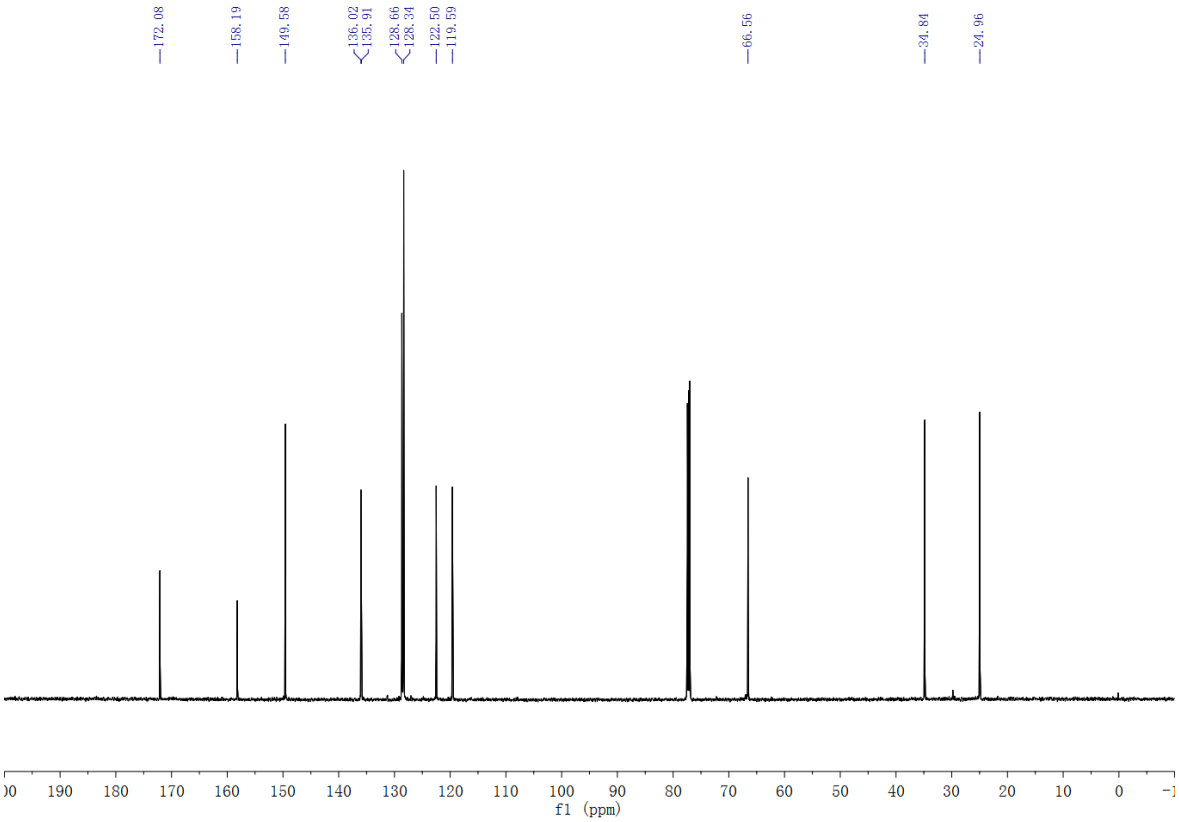


6d

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)



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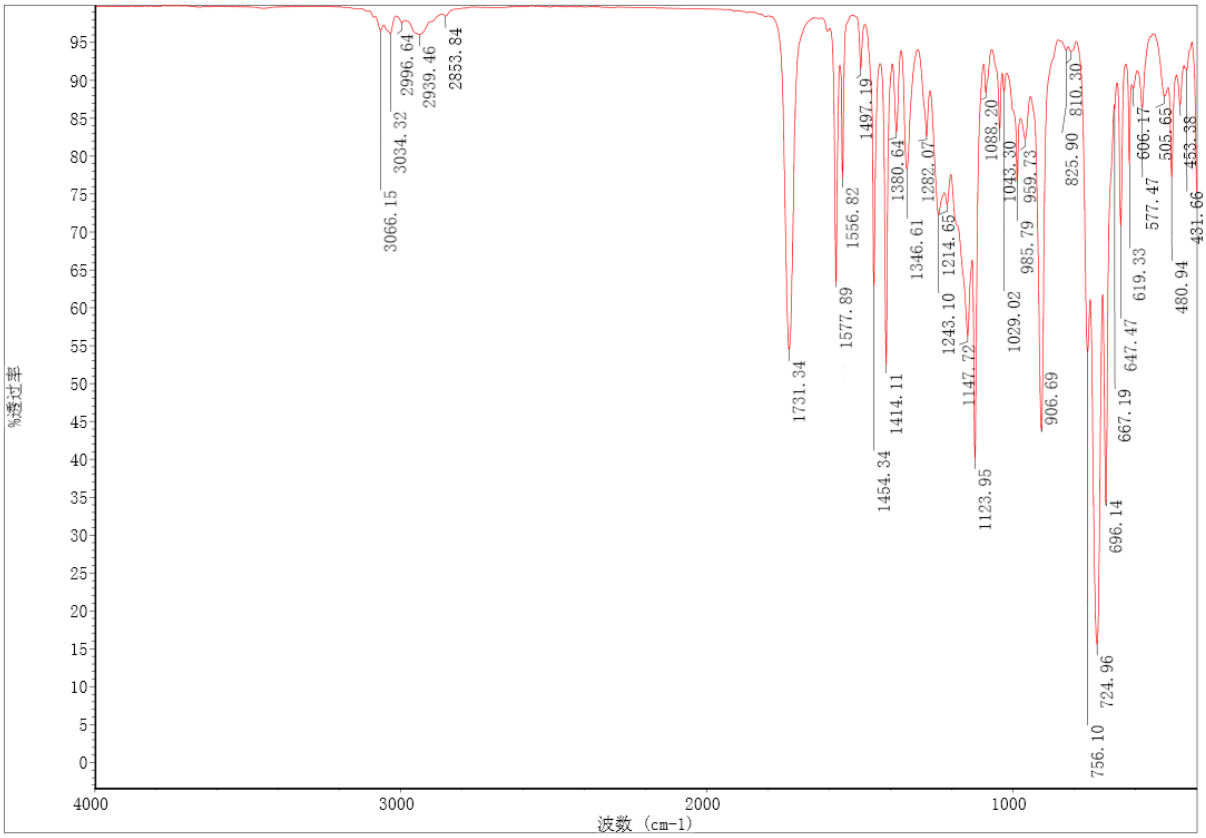
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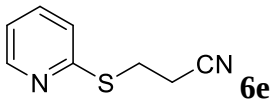
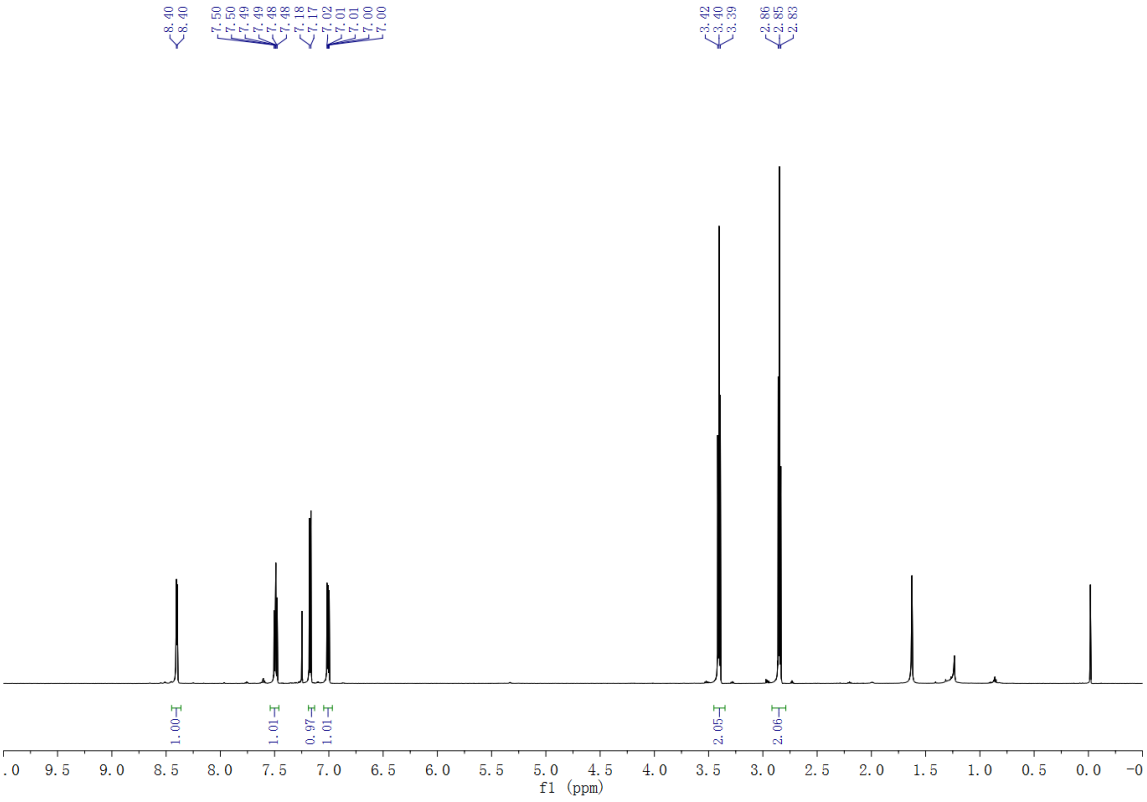
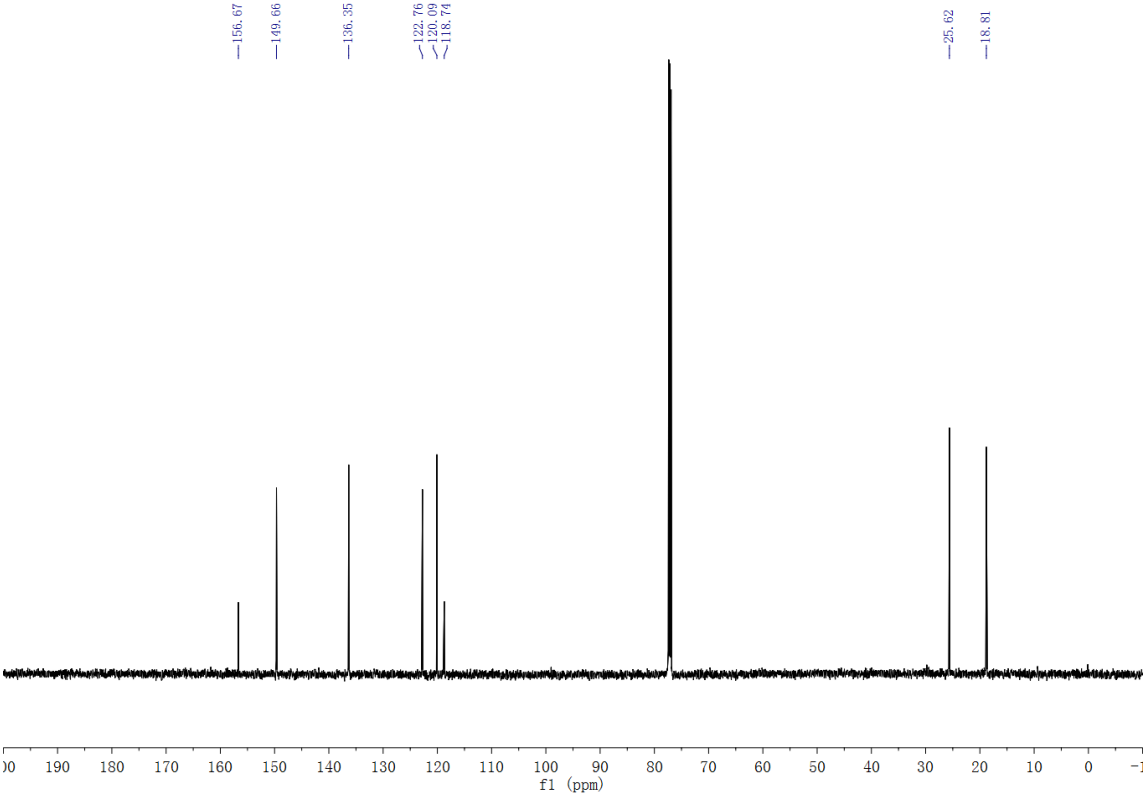


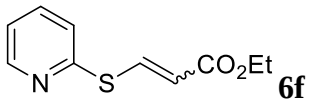
6e

^{1}H NMR ($CDCl_3$, 600 M Hz)



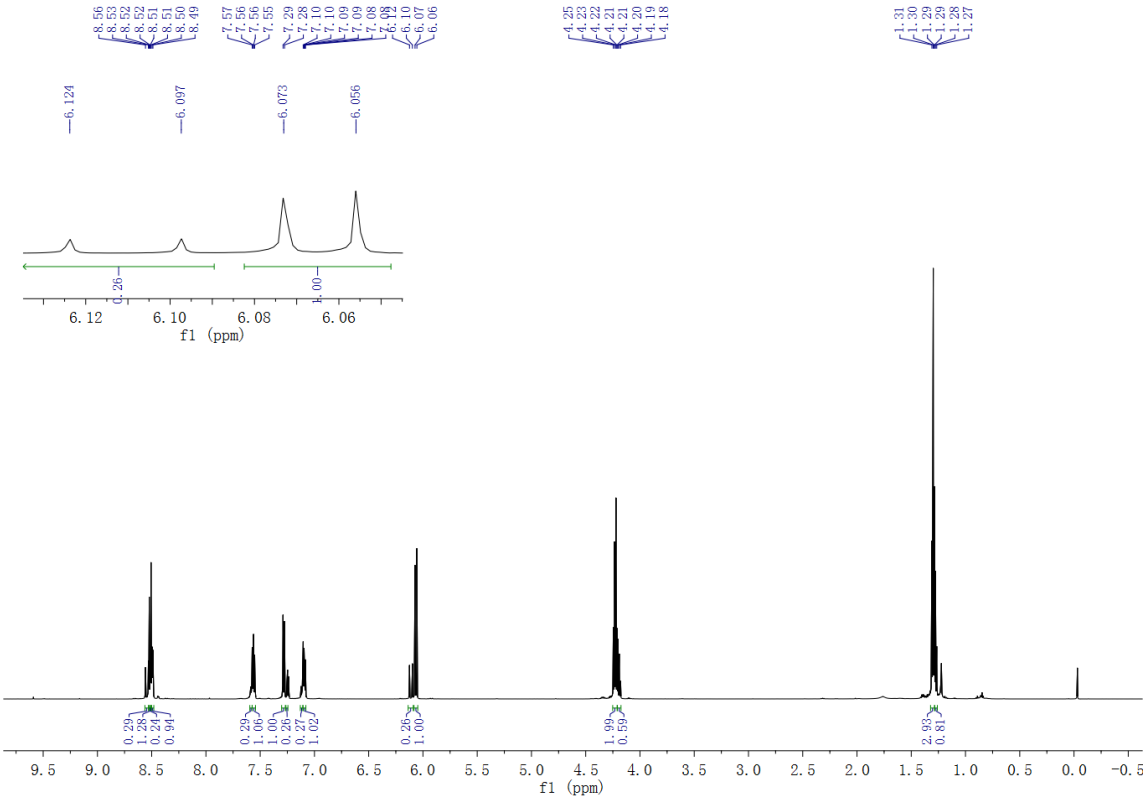
^{13}C NMR ($CDCl_3$, 150 M Hz)



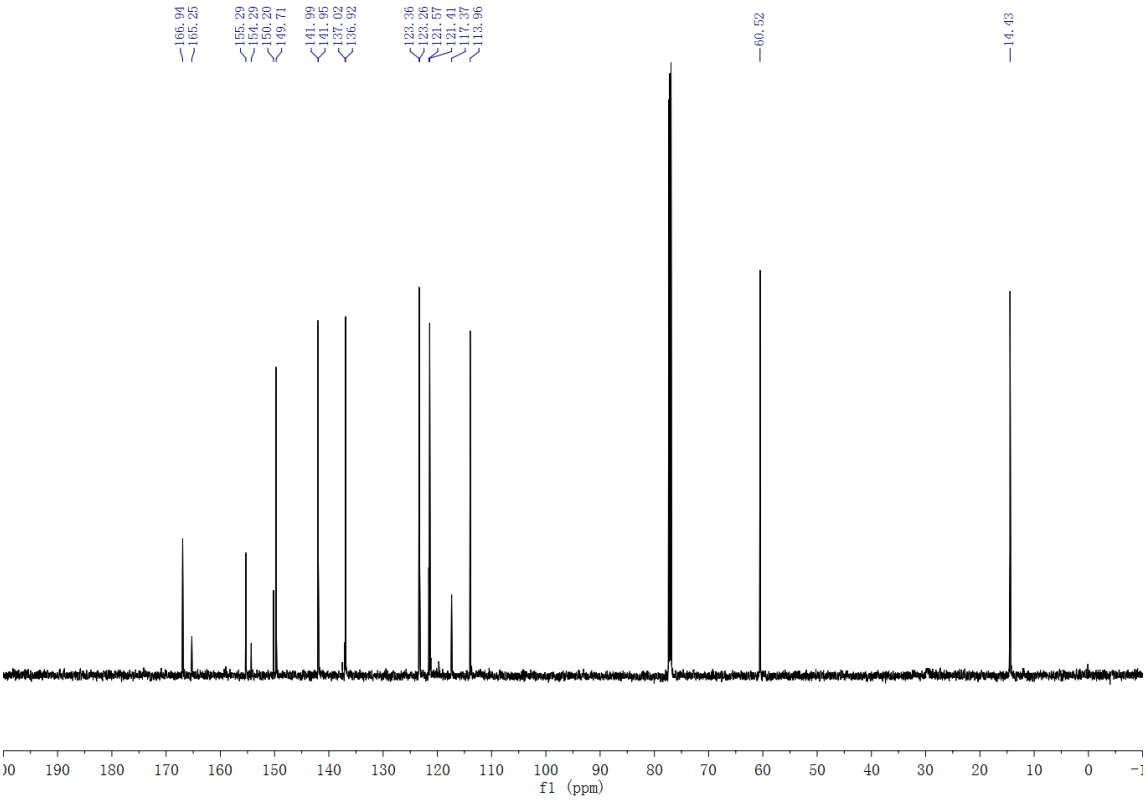


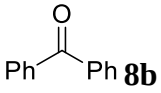
6f

^{1}H NMR ($CDCl_3$, 600 M Hz)



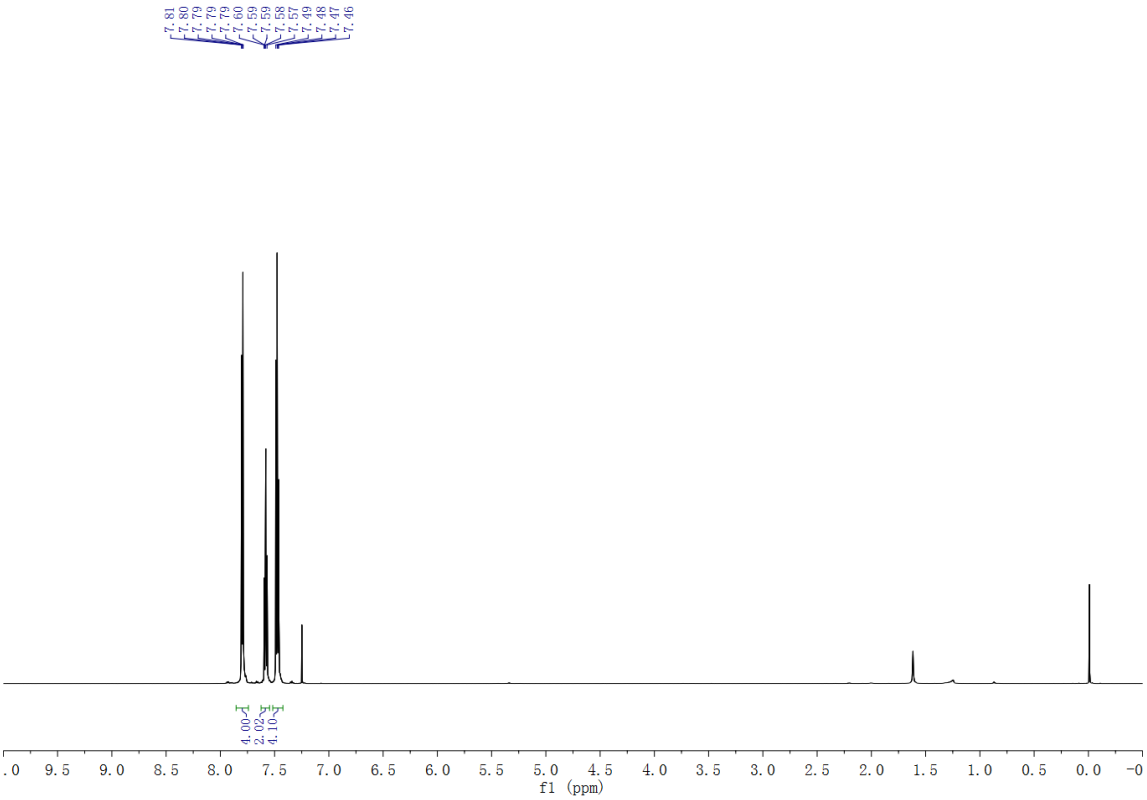
^{13}C NMR ($CDCl_3$, 150 M Hz)



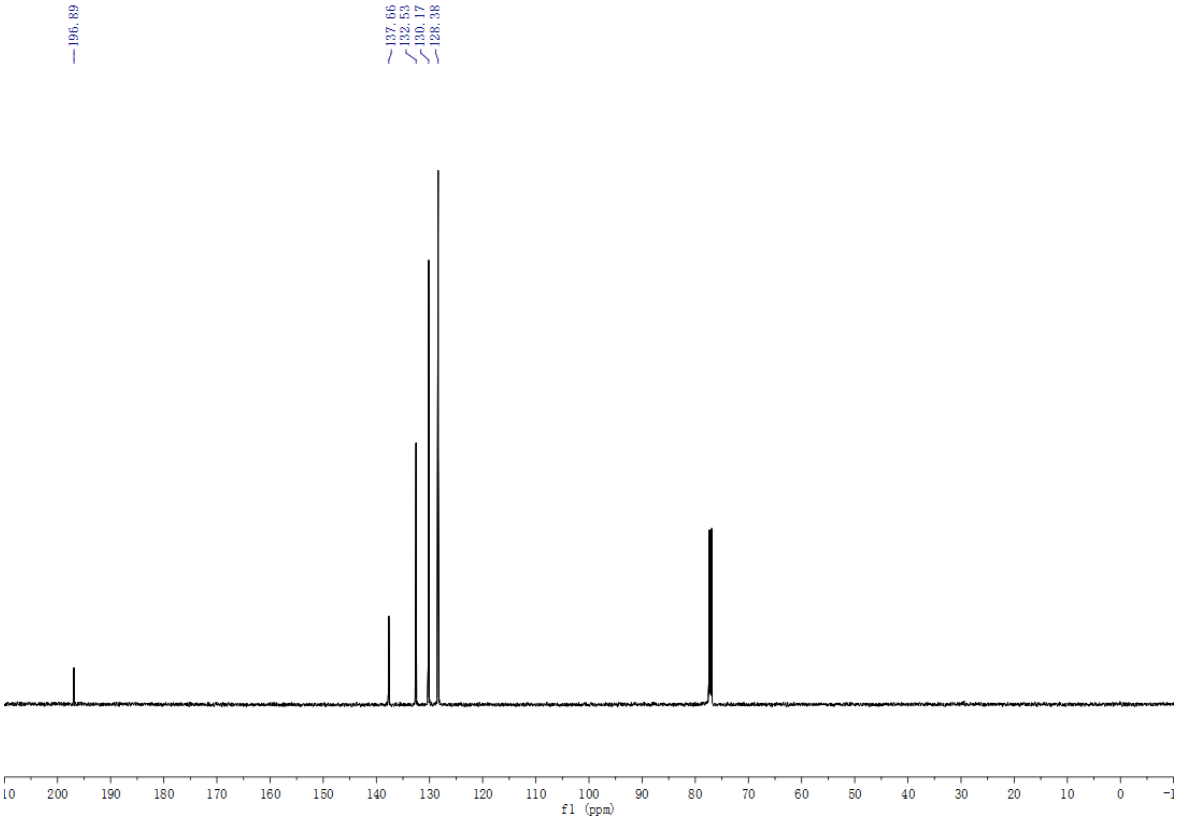


8b

^{1}H NMR ($CDCl_3$, 600 M Hz)

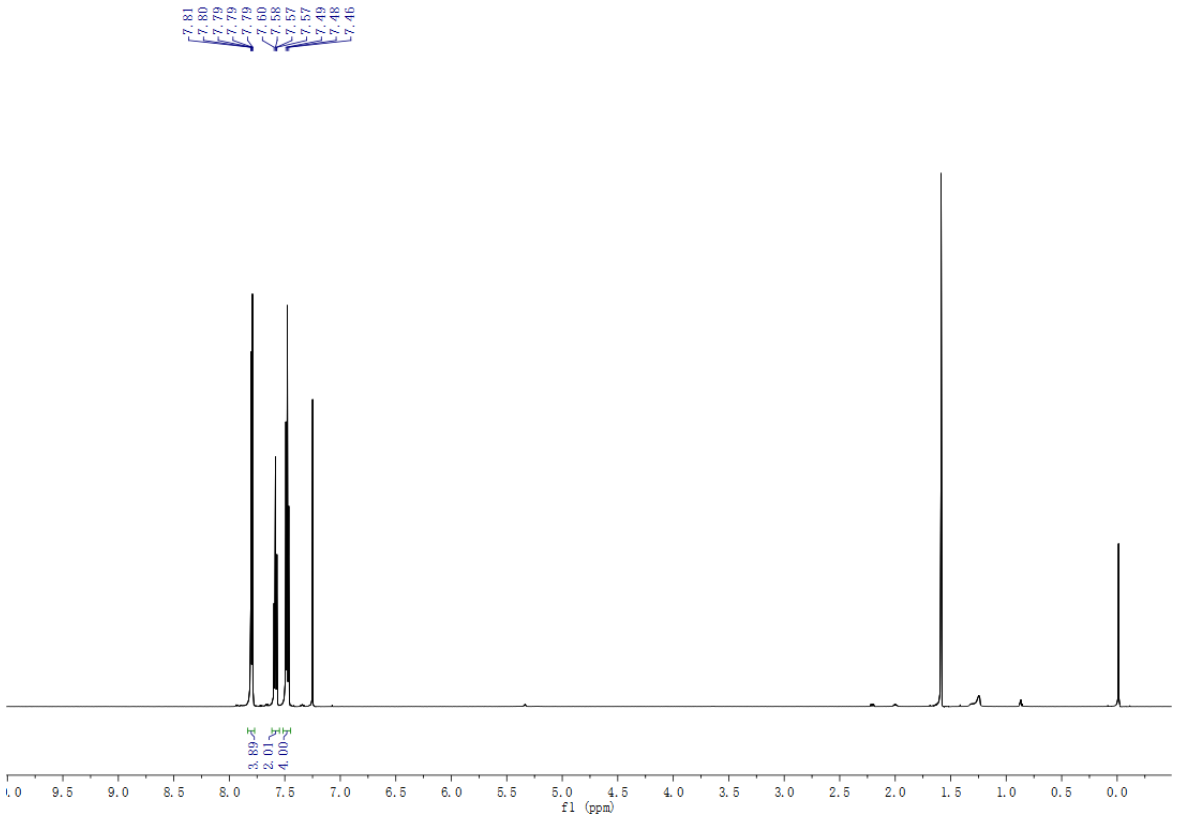


^{13}C NMR ($CDCl_3$, 150 M Hz)

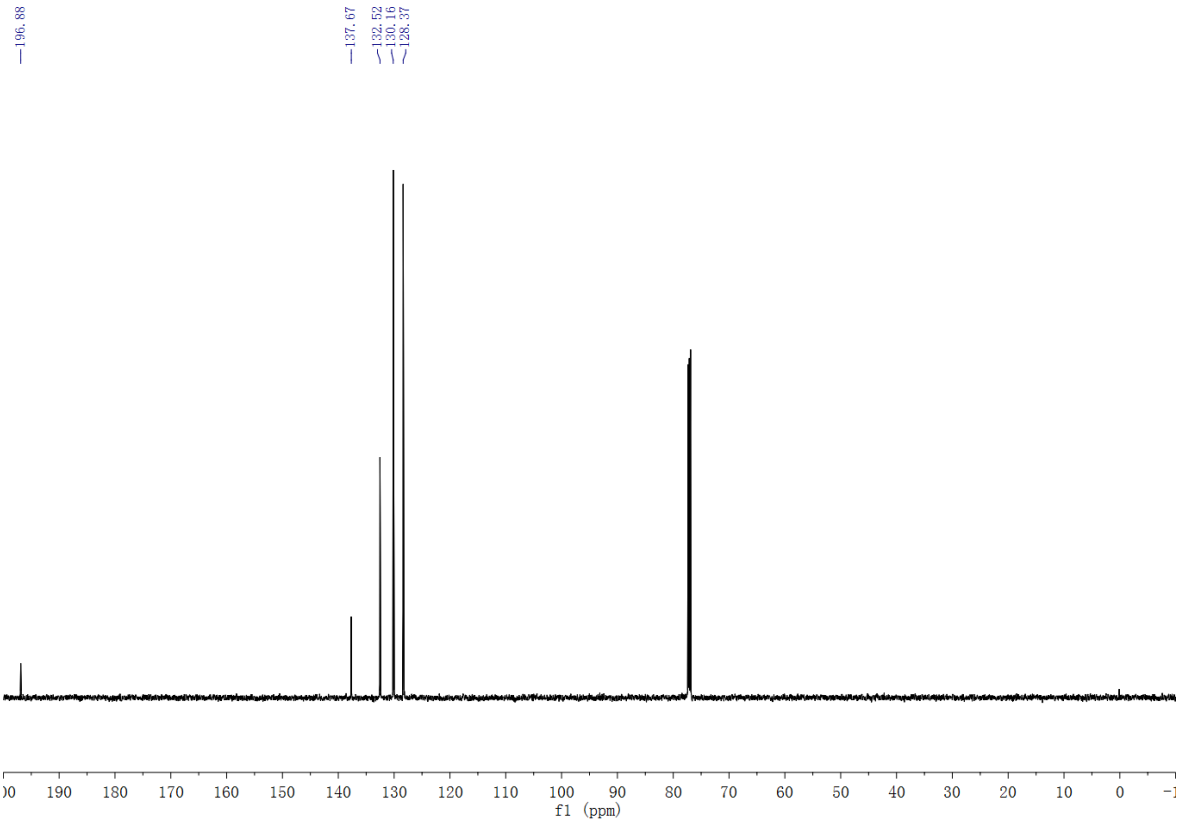


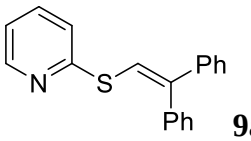
^{18}O-8b

^{1}H NMR ($CDCl_3$, 600 M Hz)



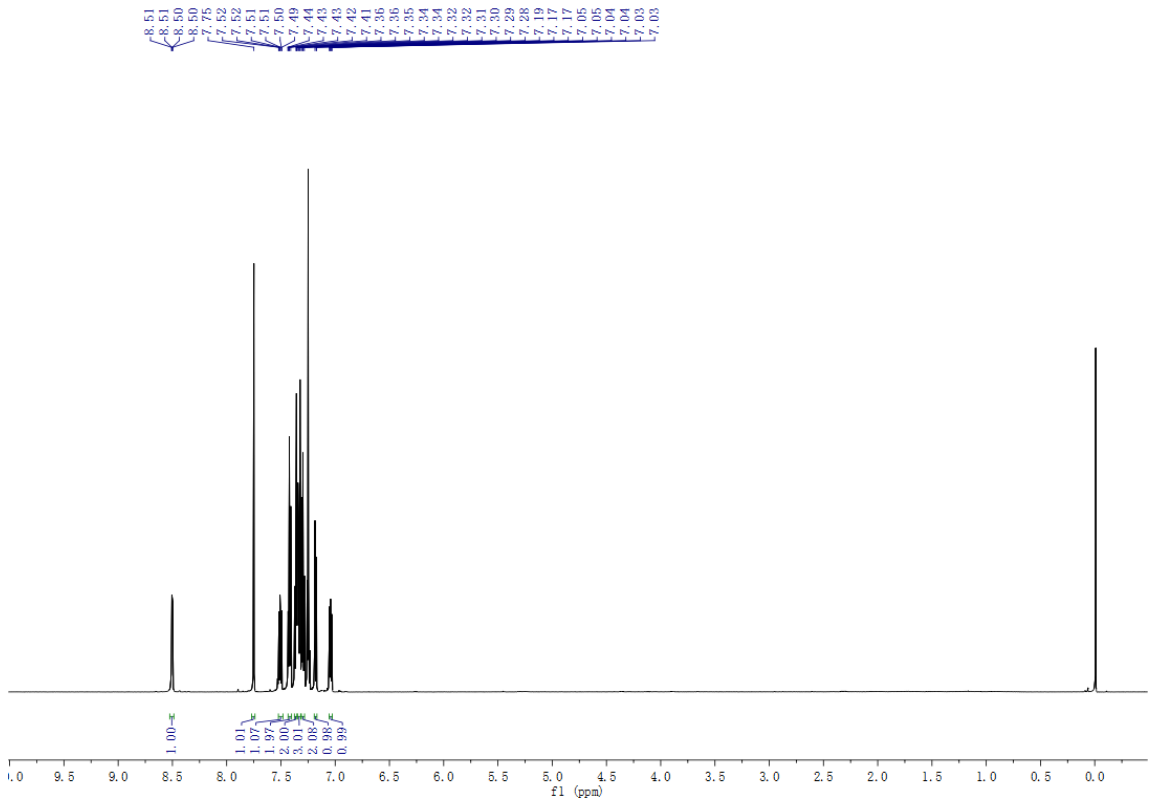
^{13}C NMR ($CDCl_3$, 150 M Hz)





9a

^{1}H NMR ($CDCl_3$, 600 M Hz)



^{13}C NMR ($CDCl_3$, 150 M Hz)